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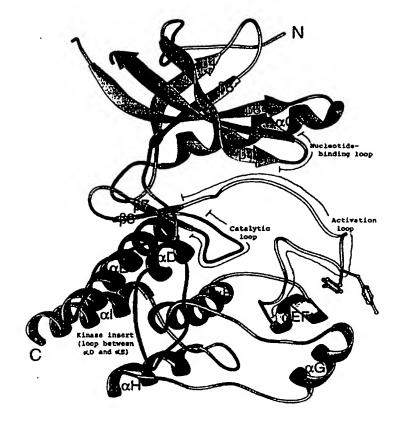
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(54) Title: CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

### (57) Abstract

The present invention relates to the threedimensional structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates that define the structures of the protein tyrosine kinase and any of the compounds bound to it are pertinent to methods for determining the three-dimensional structures of protein tyrosine kinases with unknown structure and to methods that identify modulators of protein tyrosine kinase functions.



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### DESCRIPTION

# CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

5 RELATED APPLICATIONS

This application is related to U.S. Application
Serial No. 08/701,191, by Mohammadi, et al., entitled
"Crystals of the Tyrosine Kinase Domain of Non-Insulin
Receptor Tyrosine Kinases," filed August 21, 1996 (Lyon
& Lyon Docket No. 227/088) and U.S. Application Serial
No. 60/034,168, by McMahon, et al., entitled "Crystal
Structures of a Protein Tyrosine Kinase Complexed with
Compounds of the Oxindolinone/Thiolindolinone Family,"
filed December 19, 1996 (Lyon & Lyon Docket No.
221/282), which are hereby incorporated herein by
reference in their entirety including any drawings,
tables, and figures.

### INTRODUCTION

The present invention relates to the three dimensional structures of protein kinases.

## BACKGROUND OF THE INVENTION

The following description of the background of the invention is provided simply as an aid in understanding the invention and is not admitted to describe or constitute prior art to the invention.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes (for a review, see Schlessinger and Ullrich, 1992, Neuron 9: 383-391). The PTK family contains multiple subfamilies, one of which

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is the fibroblast growth factor receptor (FGF-R) subfamily (for a review, see Givol and Yayon, 1992,  $FASEB\ J.\ 6\ (15):\ 3362-3369$ ).

All PTKs enzymatically transfer a high energy phosphate from adenosine triphosphate to a tyrosine 5 residue in a target protein. These phosphorylation events regulate cellular phenomena in signal transduction processes. Cellular signal transduction processes contain multiple steps that convert an extracellular signal into an intracellular signal. 10 intracellular signal is then converted into a cellular response. PTKs are components in many signal transduction processes. A PTK regulates the flow of a signal in a particular step in the process by phosphorylating a downstream molecule. The addition of 15 a phosphate can either modulate the activity of the downstream molecule by turning it "on" or "off". Thus, aberrations in a particular PTK's activity can either cause overflow or underflow of the signal. Overflow of a signal can lead to such abnormalities as uncontrolled 20 cell proliferation, which is representative of such

disorders as cancer and angiogenesis.

Scientists in the biomedical community are searching for PTK inhibitors that down-regulate overflow signal transduction pathways. In particular, small molecule PTK inhibitors are sought that can traverse the cell membrane and not become hydrolyzed in acidic environments. These small molecule PTK inhibitors can be highly bioavailable and can be administered orally to patients.

Some small molecule PTK inhibitors have already

been discovered. For example, bis(monocyclic), bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808), 1-cyclopropyl-4-pyridyl-quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 Al), seleoindoles and selenides (PCT WO 94/03427), tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although many PTK inhibitors are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the indolinone family, however, are specific for the FGFR subfamily and are non-hydrolyzable. WO 96/40116, "Indolinone Compounds for the Treatment of Disease," published December 19, 1996, inventors Tang et al. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, they are not complexed with PTK subfamily specific, hydrolysis resistant, small molecules.

Despite recent advances, the need remains in the art for crystallographic analysis of protein kinases, so that improved therapeutic molecules can be designed and synthesized.

### 30 SUMMARY OF THE INVENTION

The present invention relates to the three

dimensional structures of protein tyrosine kinases. The use of X-ray crystallography can define the three dimensional structure of protein tyrosine kinase at atomic resolution.

The three dimensional structures described herein 5 elucidate specific interactions between protein tyrosine kinases and compounds bound to them. The coordinates that define the three dimensional structures of protein tyrosine kinases are useful for determining three dimensional structures of PTKs with unknown structure. 10 In addition, the coordinates are also useful for designing and identifying modulators of protein tyrosine kinase function. These modulators are potentially useful as therapeutics for diseases, including (but limited to) cell proliferative diseases, such as cancer, 15 angiogenesis, atherosclerosis, and arthritis.

Thus in a first aspect, the invention features a crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

The term "crystalline form," in the context of the invention, is a crystal formed from an aqueous solution comprising a purified polypeptide corresponding to the catalytic domain of a PTK. A crystalline form of a protein tyrosine kinase is characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al., 1976, Protein Crystallography, Academic Press. A crystalline form of a protein kinase is not characterized as being capable of diffracting x-rays in a pattern analogous to a crystalline form consisting of primarily salt or primarily a compound, for example.

The term "protein tyrosine kinase," or PTK, refers to an enzyme that transfers the high energy phosphate of adenosine triphosphate to a tyrosine residue located on a protein target.

A protein tyrosine kinase catalytic domain of the invention can originate from receptor protein tyrosine kinases that bind fibroblast growth factor (FGF). These protein tyrosine kinases are known as "FGFR" herein, and can relate to one member of the FGFR family, such as FGFR1.

The term "catalytic domain" refers to the region of a protein that can exist as a separate entity from the protein. The catalytic domain of a protein tyrosine kinase is characterized as having considerable amino acid identity to the catalytic domain of other protein tyrosine kinases. Considerable amino acid identity preferably refers to at least 30% identity, more preferably at least 35% identity, and most preferably at least 40% identity. These degrees of amino acid identity refer to the identity between different protein tyrosine kinase families. Amino acid identity for members of a given protein tyrosine kinase family range from 55% to 90%. The catalytic domain may be functional as a separate entity. The catalytic domain of a protein tyrosine kinase is also characterized as a polypeptide that is soluble in solution.

The term "identity" identity as used herein refers to a property of sequences that measures their similarity or relationship. Identity is measured by dividing the number of identical residues in the two sequences by the total number of residues and

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multiplying the product by 100. Thus, two copies of exactly the same sequence have 100% identity, but sequences that are less highly conserved and have deletions, additions, or replacements have a lower degree of identity. Those skilled in the art will recognize that several computer programs are available for determining sequence identity.

The term "functional" refers to the ability of a catalytic domain to convert a substrate into a product by phosphorylating the substrate. The term "functional" also relates to the ability of a catalytic domain to bind natural binding partners. The catalytic region may comprise an N-terminal tail, a catalytic core, and a C-terminal tail. The catalytic core is a polypeptide that can be functional in terms of catalysis. N- and C-terminal tails are polypeptide regions that may not confer appreciable functionality in terms of catalysis, but may confer functionality in terms of modulator specificity.

A polypeptide can exist as a catalytic domain eventhough it is not functional. For example, a polypeptide corresponding to a catalytic domain may not be functional if it does not harbor phosphate moieties in key areas. Multiple examples of phosphorylationstate dependent function are well documented in the art. Therefore, a catalytic domain can also exist without being functional. A measure of a protein kinase catalytic domain is a polypeptide that is homologous to other protein kinase catalytic domains.

The term "polypeptide" refers to an amino acid chain representing a portion of, or the entire sequence

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of, amino acids comprising a protein.

A preferred embodiment of the invention includes a crystalline form of a PTK that is a receptor PTK.

Receptors are proteins that straddle the inside and outside of the cell membrane. Receptor PTKs comprise an extracellular region, a transmembrane region, and an intracellular region comprising a catalytic domain.

Another preferred embodiment of the invention is the crystalline form of a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

Yet another preferred embodiment of the invention is the crystalline form of a PTK that is a non-receptor PTK. Non-receptor PTKs are located inside the cell and do not harbor extracellular or membrane-spanning polypeptides attached to the polypeptide corresponding to the catalytic domain. Non-receptor PTKs may harbor fatty acids or lipids, which can impart a membrane associated character to a PTK. In preferred embodiments of the invention, crystalline forms of non-receptor PTKs are selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In still another preferred embodiment, the invention features a crystalline form of a PTK that comprises a heavy metal atom. These types of crystals can be referred to as derivative crystals.

The term "derivative crystal" refers to a crystal where the polypeptide is in association with one or more heavy-metal atoms.

The term "association" refers to a condition of proximity between a chemical entity or compound, or

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portions or fragments thereof, and tyrosine kinase domain protein, or portions or fragments thereof. The association may be non-covalent, i.e., where the juxtaposition is energetically favored by, e.g., hydrogen-bonding, van der Waals, electrostatic or hydrophobic interactions, or it may be covalent.

The term "heavy metal atom" refers to an atom that is a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

In a preferred embodiment, the invention features a crystal of an FGF receptor tyrosine kinase domain protein. The FGF receptor tyrosine kinase domain protein can relate to FGFR1.

The term "FGFR1" refers to one member of multiple receptor PTKs that are homologous to one another and bind FGF. In this context, the term "homologous" refers to at least 70% amino acid identity between two members of the FGFR family.

The term "FGFR1" can also refer to a mutant of human FGFR1 which is characterized by the amino acid sequence of SEQ ID NO:2. As compared to human FGFR1, FGFR1 contains the following amino acid substitutions: Cys-488 - Ala, Cys-584 - Ser, Leu-457 - Val, and has an additional five amino acid residues at the N-terminus (Ser-Ala-Ala-Gly-Thr).

The term "human FGFR1" refers to the tyrosine

kinase domain of human fibroblast growth factor receptor

("FGFR1") having the amino acid sequence of SEQ ID

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NO:1. Generally, human FGFR1 comprises a 310 amino acid residue fragment (residues 456 to 765) of human FGFR1.

The term "mutant" refers to a polypeptide which is obtained by replacing at least one amino acid residue in a native tyrosine kinase domain with a different amino acid residue. Mutation can be accomplished by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native tyrosine kinase domain having substantially the same three-dimensional structure as the native tyrosine kinase domain from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the  $C\alpha$  atoms of the native tyrosine kinase are included in the superposition. A mutant may have, but need not have, PTK activity.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 1.

25 The term "atomic structural coordinates" as used herein refers to a data set that defines the three dimensional structure of a molecule or molecules.

Structural coordinates can be slightly modified and still render nearly identical three dimensional

30 structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the

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resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed by a person of ordinary skill in the art as identical. Hence, the structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 are not limited to the values defined therein.

In other preferred embodiments, the invention features a crystalline form of the polypeptide in association with a compound. These types of crystalline forms can be referred to as co-crystals. The compound may be a cofactor, substrate, substrate analog, inhibitor, or allosteric effector.

The term "compound" refers to an organic molecule.

The term "organic molecule" refers to a molecule which has at least one carbon atom in its structure. The compound can have a molecular weight of less than 6kDa. Both the geometry of the compound and the interactions formed between the compound and the polypeptide

preferably govern high affinity binding between the two molecules. High affinity binding is preferably governed by a dissociation equilibrium constant on the order of 10-6 M or less. The compound is preferably a modulator that alters the function of a PTK.

The term "function," in reference to the effect of a modulator on PTK function, refers to the ability of a modulator to enhance or inhibit the catalytic activity of a PTK.

The term "catalytic activity", in the context of
the invention, defines the ability of a PTK to
phosphorylate a substrate polypeptide. Catalytic

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activity can be measured, for example, by determining the amount of a substrate converted to a product as a function of time. The conversion of the substrate to a product occurs at the active-site of the PTK.

The term "active-site" refers to a cavity located in the PTK in which one or more substrate molecules may bind. Addition of a modulator to cells expressing a PTK may enhance (activate) or lower (inhibit) the catalytic activity of the PTK.

A small number of inhibitors of PTK catalytic activity are known in the art. Small molecule inhibitors may modulate PTK function by blocking the binding of substrates. Indolinone compounds, for example, may bind to the active-site of PTK catalytic domains and inhibit them effectively, as measured by inhibition constants on the order of 10.6 M or less.

Activators of PTK intracellular regions can enhance PTK function by interacting with both the PTK catalytic domain and the substrate. Activators may also promote dimerization of PTKs and thus activate them by bringing them into close proximity with one another. In addition, activators may operate by promoting a conformational change in the intracellular region of the PTK such that the catalytic region modifies substrates at a faster rate in the presence of the activator.

The term "function" can also refer to the ability of a modulator to enhance or inhibit the association between a PTK and a natural binding partner.

The term "natural binding partner" refers to a polypeptide that normally binds to a PTK in a cell.

These natural binding partners can play a role in

propagating a signal in a PTK signal transduction process. The natural binding partner can bind to a PTK with high affinity. High affinity represents an equilibrium binding constant on the order of  $10^{-6}\ \mathrm{M}$  or less. However, a natural binding partner can also transiently interact with a PTK and chemically modify PTK natural binding partners are chosen from a group consisting of, but not limited to, src homology 2 (SH2) or 3 (SH3) domains, other phosphoryl tyrosine

binding (PTB) domains, nucleotide exchange factors, and other protein kinases or protein phosphatases. The term "interactions" refers to hydrophobic, aromatic, and ionic forces and hydrogen bonds formed between atoms in the modulator and the enzyme active-

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The term "cofactor" refers to a compound that may, in addition to the substrate, bind to a protein and undergo a chemical reaction. Multiple co-factors are nucleotides or nucleotide derivatives, such as phosphate and nicotinamide derivatives of adenosine.

The term "substrate" refers to a compound that reacts with an enzyme. Enzymes can catalyze a specific reaction on a specific substrate. For example, PTKs can phosphorylate specific protein and peptide substrates on tyrosine moieties. In addition, nucleotides can act as substrates for protein kinases.

The term "substrate analog" refers to a compound that is structurally similar, but not identical, to a substrate. The substrate analog may be a nucleotide analog. Examples of nucleotide analogs are described below.

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The term "inhibitor" refers to a compound that decreases the cellular function of a protein kinase. The protein kinase function is preferably the interaction with a natural binding partner and more preferably catalytic activity.

The term "allosteric effector" refers to a compound that causes allosteric interactions in a protein. The term "allosteric interactions" refers to interactions between separate sites on a protein. The sites can be different from the active site. The allosteric effector can enhance or inhibit catalytic activity by binding to a site that may be different than the active site.

The term "co-crystal" refers to a crystal where the polypeptide is in association with one or more compounds.

In preferred embodiments, a co-crystal of the invention can be in association with a heavy metal atom. Examples of heavy metal atoms are described above.

In other preferred embodiments, the invention features a co-crystal comprising the crystalline form of the polypeptide in association with a compound, where the compound is a non-hydrolyzable analog of ATP. These analogs can be referred to as nucleotide analogs.

The term "ATP" refers to the chemical compound adenosine triphosphate.

The term "non-hydrolyzable" refers to a compound having a covalent bond that does not readily react with water. Examples of non-hydrolyzable analogs of ATP are AMP-PNP and AMP-PCP, whose structures are well known to those skilled in the art.

The term "AMP-PNP" refers to adenylyl

imidodiphosphate, a non-hydrolyzable analog of ATP.

The term "AMP-PCP" refers to adenylyl diphosphonate, a non-hydrolyzable analogue of ATP.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 2.

In preferred embodiments, the invention relates to crystalline forms, where the compound in association with the polypeptide is an indolinone.

Certain indolinones are specific modulators of PTK function. A preferred embodiment of the invention is the crystalline form of a PTK complexed with an indolinone of formula I or II:

$$R_{5}$$
 $R_{6}$ 
 $R_{7}$ 
 $R_{1}$ 
 $R_{4}$ 
 $R_{4}$ 
 $R_{5}$ 
 $R_{6}$ 
 $R_{6}$ 
 $R_{7}$ 
 $R_{1}$ 

$$R_5$$
 $A_2$ 
 $A_1$ 
 $R_6$ 
 $A_3$ 
 $A_4$ 
 $R_7$ 
 $R_1$ 
 $R_1$ 
 $R_2$ 
 $R_1$ 
 $R_1$ 
 $R_2$ 
 $R_1$ 
 $R_1$ 
 $R_2$ 

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, where:

- (a)  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are independently carbon or nitrogen;
  - (b) R<sub>1</sub> is hydrogen or alkyl;
  - (c)  $R_2$  is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
    - (d) R<sub>3</sub> is hydrogen;
- (e) R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> are optionally present, and are either (i) independently selected from the group consisting of alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R, and CONRR' or (ii) any two adjacent R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> taken together form a fused ring with the aryl portion of the indole-based portion of the indolinone;
- (f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each
  independently selected from the group consisting of
  hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl,
  alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R,
  SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R,

and CONRR';

- (g) n is 0, 1, 2, or 3;
- (h) R is hydrogen, alkyl or aryl;
- (i) R' is hydrogen, alkyl or aryl; and
- 5 (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-
- oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 10 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, 15
- alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R or CONRR'.

The term "pharmaceutically acceptable salt" refers to those salts which retain the biological activity and 20 properties of the free bases. Pharmaceutically acceptable salts can be obtained by reaction with inorganic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid, methanesulfonic acid, ethanesulfonic acid, p-

25 toluenesulfonic acid, salicylic acid and the like.

The term "prodrug" refers to an agent that is converted into the parent drug in vivo. Prodrugs may be easier to administer than the parent drug in some situations. For example, the prodrug may be bioavailable by oral administration but the parent is not, or the prodrug may improve solubility to allow for

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intravenous administration.

"Alkyl" refers to a straight-chain, branched or cyclic saturated aliphatic hydrocarbon. Preferably, the alkyl group has 1 to 12 carbons. More preferably, it is a lower alkyl of from 1 to 7 carbons, more preferably 1 to 4 carbons. Typical alkyl groups include methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tertiary butyl, pentyl, hexyl and the like. The alkyl group may be optionally substituted with one or more substituents are selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkenyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon group containing at least one carbon-carbon double bond. Preferably, the alkenyl group has 2 to 12 carbons. More preferably it is a lower alkenyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkenyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkynyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon containing at least one carbon-carbon triple bond. Preferably, the alkynyl group has 2 to 12 carbons. More preferably it is a lower alkynyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkynyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO<sub>2</sub>, halogen, N(CH<sub>3</sub>)<sub>2</sub> amino, and SH.

"Alkoxy" refers to an "O-alkyl" group.

"Aryl" refers to an aromatic group which has at least one ring having a conjugated pi-electron system and includes carbocyclic aryl, heterocyclic aryl and biaryl groups. The aryl group may be optionally

substituted with one or more substituents selected from the group consisting of halogen, trihalomethyl, hydroxyl, SH, OH, NO<sub>2</sub>, amine, thioether, cyano, alkoxy, alkyl, and amino.

"Alkaryl" refers to an alkyl that is covalently joined to an aryl group. Preferably, the alkyl is a lower alkyl.

"Carbocyclic aryl" refers to an aryl group wherein the ring atoms are carbon.

"Heterocyclic aryl" refers to an aryl group having from 1 to 3 heteroatoms as ring atoms, the remainder of the ring atoms being carbon. Heteroatoms include oxygen, sulfur, and nitrogen. Thus, heterocyclic aryl groups include furanyl, thienyl, pyridyl, pyrrolyl, N-lower alkyl pyrrolo, pyrimidyl, pyrazinyl, imidazolyl and the like.

"Amide" refers to -C(0)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Thioamide" refers to -C(S)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Amine" refers to a -N(R')R'' group, where R' and R'' are independently selected from the group consisting of alkyl, aryl, and alkylaryl.

"Thioether" refers to -S-R, where R is alkyl, aryl, or alkylaryl.

"Sulfonyl" refers to -S(O)<sub>2</sub>-R, where R is aryl, C(CN)=C-aryl, CH<sub>2</sub>CN, alkyaryl, sulfonamide, NH-alkyl, NH-

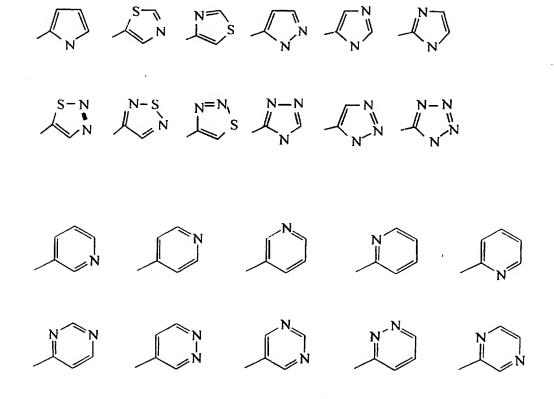


alkylaryl, or NH-aryl.

The term "acyl" denotes groups -C(0)R, where R is alkyl as defined above, such as formyl, acetyl, propionyl, or butyryl.

It is understood by those skilled in the art that when  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are nitrogen or sulfur that the corresponding  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$ , as well as the corresponding bond, do not exist.

Examples of indoles having such fused rings (as described in (e) (ii) above include the following:



The six membered rings shown above exemplify possible A rings in compound II.

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Other preferred embodiments of the invention are crystalline forms comprising 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone as well as 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone. The polypeptide of these crystalline forms can be FGFR, and specifically, FGFR1.

In preferred embodiments, the crystalline forms of the invention can be defined by the structural coordinates set forth in Table 3 or Table 4.

The use of X-ray crystallography can elucidate the three dimensional structure of crystalline forms of the invention. The first characterization of crystalline forms by X-ray crystallography can determine the unit cell shape and its orientation in the crystal.

In other preferred embodiments, the invention features a crystal of an FGF receptor tyrosine kinase domain protein, where the crystal is characterized by having monoclinic unit cells. The crystal may also be characterized by having space group symmetry C2.

The term "unit cell" refers to the smallest and simplest volume element (i.e., parallelpiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The dimensions of the unit cell are defined by six numbers: dimensions a, b and c and angles  $\alpha$ ,  $\beta$  and  $\gamma$ . A crystal can be viewed as an efficiently packed array of multiple unit cells. Detailed descriptions of crystallographic terms are described in, which is hereby incorporated herein by reference in its entirety, including any drawings, figures, and tables.

The term "monoclinic unit cell" refers to a unit

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cell where a  $\neq$  b  $\neq$  c;  $\alpha$  =  $\gamma$  = 90°; and  $\beta$  > 90°...

The term "space group" refers to the symmetry of a unit cell. In a space group designation (e.g., C2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance.

The term "lattice" in reference to crystal structures refers to the array of points defined by the vertices of packed unit cells.

The term "symmetry operations" refers to geometrically defined ways of exchanging equivalent parts of a unit cell, or exchanging equivalent molecules between two different unit cells. Examples of symmetry operations are screw axes, centers of inversion, and mirror planes.

In a preferred embodiment, the invention features a crystalline form, where the monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and  $\beta$ =107.2°.

In a preferred embodiment, the invention features a FGFR1 crystal, where the monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and  $\beta$ =107.7°.

In another aspect the invention features a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal

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boundary of the catalytic domain.

The polypeptides of the invention can be isolated, enriched or purified. In addition, the crystalline forms of the invention can be formed from polypeptides that are isolated, enriched, or purified.

By "isolated" in reference to a polypeptide is meant a polymer of 6, 12, 18 or more amino acids conjugated to each other, including polypeptides that are isolated from a natural source or that are synthesized. The isolated polypeptides of the present invention are unique in the sense that they are not found in a pure or separated state in nature. Use of the term "isolated" indicates that a naturally occurring sequence has been removed from its normal cellular environment. Thus, the sequence may be in a cell-free solution or placed in a different cellular environment. The term does not imply that the sequence is the only amino acid chain present, but that it is essentially free (about 90 - 95% pure at least) of material naturally associated with it

By the use of the term "enriched" in reference to a polypeptide it is meant that the specific amino acid sequence constitutes a significantly higher fraction (2 - 5 fold) of the total of amino acids present in the cells or solution of interest than in normal or diseased cells or in the cells from which the sequence was taken. This could be caused by a person by preferential reduction in the amount of other amino acids present, or by a preferential increase in the amount of the specific amino acid sequence of interest, or by a combination of the two. However, it should be noted that "enriched"

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does not imply that there are no other amino acid sequences present, just that the relative amount of the sequence of interest has been significantly increased. The term significant here is used to indicate that the level of increase is useful to the person making such an increase, and generally means an increase relative to other amino acids of about at least 2 fold, more preferably at least 5 to 10 fold or even more. The term also does not imply that there are no amino acids from other sources. The other source amino acids may, for example, comprise amino acids encoded by a yeast or bacterial genome, or a cloning vector such as pUC19. The term is meant to cover only those situations in which a person has intervened to elevate the proportion of the desired nucleic acid.

It is also advantageous for some purposes that an amino acid sequence be in purified form. The term "purified" in reference to a polypeptide does not require absolute purity (such as a homogeneous preparation); instead, it represents an indication that the sequence is relatively purer than in the natural environment (compared to the natural level this level should be at least 2-5 fold greater, e.g., in terms of mg/ml). Purification of at least one order of magnitude, preferably two or three orders, and more preferably four or five orders of magnitude is expressly contemplated. The substance is preferably free of contamination at a functionally significant level, for example 90%, 95%, or 99% pure.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a

receptor PTK. The receptor PTK may have a threedimensional structure substantially similar to that of the insulin receptor, even though the amino acid content may be different.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, where the non-insulin receptor tyrosine kinase is a cytoplasmic tyrosine kinase.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a receptor PTK, selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, or MUSK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, or ACK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a PTK, having the amino acid sequence shown in Table 1 or Table 2.

In another aspect, the invention features a method for creating crystalline forms described herein. The method may utilize the polypeptides described herein to form a crystal. The method comprises the steps of:

- (a) mixing a volume of polypeptide solution with a reservoir solution; and
- (b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container, under conditions suitable for crystallization.

These processes are described in detail in the

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section entitled "Detailed Description of the Invention."

In another aspect, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of: (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, where the polypeptide solution comprises 1 mg/mL to 60 mg/mL FGFtype tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and where the reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v)ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and (b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25°C until crystals form.

In a preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

In another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine

kinase domain polypeptide in crystalline form, where the polypeptide solution includes a compound such as a cofactor, substrate, substrate analog, inhibitor or allosteric effector.

In still another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the compound is a nucleotide analog, such as a non-hydrolyzable analog of ATP, or an indolinone.

Indolinone compounds have the general structural formula as described herein.

In another aspect, the invention features a cDNA encoding an FGF receptor tyrosine kinase domain protein, where a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.

Another aspect of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by utilizing the structural coordinates of Table 1, Table 2, Table 3, and Table 4. These methods can relate to homology modeling, molecular replacement, and nuclear magnetic resonance methods.

In a preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structures by utilizing the coordinates of Table 1, Table 2, Table 3, or Table 4 in conjunction with the amino acid sequences of PTKs. This method of homology modeling comprises the steps of: (a)

aligning the computer representation of an amino acid sequence of a PTK with unknown structure with that of a PTK with known structure, where alignment is achieved by matching homologous regions of the amino acid sequences;

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(b) transferring the computer representation of an amino acid structure in the PTK sequence of known structure to a computer representation of a structure of the corresponding amino acid in the PTK sequence with unknown structure; and (c) determining low energy conformations of the resulting PTK structure.

The term "amino acid sequence" describes the order of amino acids in the amino acid chain comprising a polypeptide corresponding to the catalytic domain of a PTK.

The term "aligning" describes matching the beginning and the end of two or more amino acid sequences. Homologous amino acid sequences are placed on top of one another during the alignment process.

The term "homologous" describes amino acids in two sequences that are identical or have similar side-chain chemical groups (e.g., aliphatic, aromatic, polar, negatively charged, or positively charged).

The term "corresponding" refers to an amino acid that is aligned with another in the sequence alignment mentioned above.

The term "determining the low energy conformation" describes a process of changing the conformation of the PTK structure such that the structure is of low free energy. The PTK structure may or may not have molecules, such as modulators bound to it.

The term "low free energy" describes a state where the molecules are in a stable state as measured by the process. A stable state is achieved when favorable interactions are formed within the complex.

The term "favorable interactions" refers to

hydrophobic, aromatic, and ionic forces, and hydrogen bonds.

Another preferred embodiment of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure. This method is accomplished by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to an incomplete X-ray crystallographic data set for a PTK. The method comprises the steps of: (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals, where one data set is complete and the other is incomplete; and (b) determining a low energy conformation of the resulting PTK structure.

The term "incomplete data set" relates to a X-ray crystallographic data set that does not have enough information to give rise to a three dimensional structure.

In another preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to nuclear magnetic resonance (NMR) data of a PTK. This method comprises the steps of: (a)

determining the secondary structure of a PTK structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The PTK structure may not be complexed with compounds or modulators.

The term "secondary structure" describes the arrangement of amino acids in a three dimensional

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structure, such as in  $\alpha$ -helix or  $\beta$ -sheet elements.

The term "through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence.

The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

In another aspect, the invention features a method of identifying potential modulators of PTK function.

These modulators are identified by docking a computer representation of a structure of a compound with a computer representation of a cavity formed by the active-site of a PTK. The computer representation of the PTK active-site structure can be defined by structural coordinates.

The term "chemical group" refers to moieties that can form hydrogen bonds, hydrophobic, aromatic, or ionic interactions.

The term "docking" refers to a process of placing a compound in close proximity with a PTK. The term can also refer to a process of finding low energy conformations of the compound/PTK complex.

A preferred embodiment of the invention is a method of identifying potential modulators of PTK function.

The method involves utilizing the structural coordinates or a PTK three dimensional structure. The structural coordinates set forth in Table 1, Table 2, Table 3, and

Table 4 can be utilized. The method comprises the steps of: (a) removing a computer representation of a PTK

structure and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the PTK; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying compounds that best fit the PTK active-site as potential modulators of PTK function. The initial PTK structure may or may not have compounds bound to it.

The term "favorable geometric fit" refers to a conformation of the compound-PTK complex where the surface area of the compound is in close proximity with the surface area of the active-site without forming unfavorable interactions. Unfavorable interactions can be steric hindrances between atoms in the compound and atoms in the PTK active-site.

The term "favorable complementary interactions" relates to hydrophobic, aromatic, ionic, and hydrogen bond donating, and hydrogen bond accepting forces formed between the compound and the PTK active-site.

The term "potential" qualifies the term "modulator of PTK function" because the potential modulator or PTK function has not yet been tested for activity in vitro or in vivo.

The term "best fit" describes compounds that complexed the most surface area in the complex and/or form the most favorable complementary interactions with the PTK in the screen in a given experiment.

Another preferred embodiment of the invention is a method of identifying potential modulators of PTK function. The method involves utilizing a three

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dimensional structure of a PTK, with or without compounds bound to it. The method comprises the steps of: (a) modifying a computer representation of a PTK having one or more compounds bound to it, where the computer representations of the compound or compounds and PTK are defined by structural coordinates; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying the compounds that best fit the PTK active-site as potential modulators of PTK function.

The term "modifying" relates to deleting a chemical group or groups or adding a chemical group or groups.

Computer representations of the chemical groups can be selected from a computer data base.

Yet another preferred embodiment of the invention is a method of identifying potential modulators of PTK function by operating modulator construction or modulator searching computer programs on the compounds complexed with the PTK. The method comprises the steps of: (a) removing a computer representation of one or more compounds complexed with a PTK; and (b) searching a data base for compounds similar to the removed compounds using a compound searching computer program, or replacing portions of the compounds complexed with the PTK with similar chemical structures from a data base using a compound construction computer program, where the representations of the compounds are defined by structural coordinates.

The term "operating" as used herein refers to utilizing the three-dimensional conformation of

molecules defined by the processes described herein in various computer programs.

The term "similar compound" refers to a compound in a computer data base that has a similar geometric structure as compounds that can bind to a PTK. The similar compound can also have similar chemical groups as the compounds that are either bound to the PTK or once bound to the PTK. The similar chemical groups can form complementary interactions with the PTK.

The term "compound searching computer program"

describes a computer program that searches computer
representations of compounds from a computer data base
that have similar three dimensional structures and
similar chemical groups as a compound of interest. The
compound of interest is preferably an indolinone
compound.

The term "similar chemical structures" refers to chemical groups that share similar geometry as portions of the compounds in complex with the PTK or compounds removed from the PTK structure. Similar chemical structures can also refer to chemical groups that may form similar complementary interactions as portions of the compounds in complex with the PTK or compounds removed from the PTK structure.

The term "replacing structures" refers to removing a portion of the compounds in complex with the PTK or compounds removed from the PTK structure and connecting the broken bonds to a similar chemical structure.

The term "compound construction computer program"

describes a computer program that replaces computer
representations of chemical groups in a compound with

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groups from a computer data base. The compound is preferably an indolinone compound.

The term "similar three dimensional structure" describes two molecules with nearly identical shape and volume.

In another preferred embodiment of the invention, the PTK structures used in the modulator design or identification method of the invention are defined by the structural coordinates of Table 1, Table 2, Table 3, or Table 4.

The methods for using the crystalline forms and three dimensional structures of the invention can relate to a broad range of protein kinases. Thus, in preferred embodiments, the invention relates to a receptor PTK. The receptor PTK can be selected form the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. The PTK may also exist as a non-receptor PTK. The non-receptor PTK can be selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In another aspect, the invention features a potential modulator of PTK function identified by methods disclosed in the invention.

A preferred embodiment of the invention is that the potential modulator of PTK function is an oxindolinone or a thiolindolinone of formula I or II disclosed above.

Another aspect of the invention is a method for synthesizing a potential modulator of PTK function or its pharmaceutically acceptable salts, isomers, metabolites, esters, amides, or prodrugs by a standard

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synthetic method known in the art. Synthetic procedures are discussed below.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of PTK phosphorylation between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in the level of PTK phosphorylation.

The term "cells" refers to any type of cells either primary or cultured. Primary cells can be extracted directly from an organism while cultured cells rapidly divide and can be cultured in many successive rounds. Cells can be grown in a variety of containers including, but not limited to flasks, dishes, and well plates.

The term "administer" refers to a method of delivering a compound to cells. The compound can be prepared using a carrier such as dimethyl sulfoxide (DMSO) in an aqueous solution. The aqueous solution comprising the compound, also termed an "aqueous preparation", can be simply mixed into the medium bathing the layer of cells or microinjected into the cells themselves. The compounds may be administered to the cells using a suitable buffered solution.

The term "suitable buffered solution" refers to an aqueous preparation of the compound that comprises a salt that can control the pH of the solution at low concentrations. Because the salt exists at low

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concentrations, the salt preferably does not alter the function of the cells.

The term "PTK phosphorylation" refers to the presence of phosphate on the PTK. Phosphates on PTKs can be identified by antibodies that bind them specifically with high affinity.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of cell growth between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in cell growth.

The term "cell growth" refers to the rate at which a group of cells divides. Cell division rates can be readily measured by methods utilized by those skilled in the art.

Another aspect of the invention features a method of diagnosing a disease by identifying cells harboring a PTK with inappropriate activity. The method comprises the steps of: (a) administering a modulator of PTK function to cells; (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and (c) diagnosing a disease by characterizing cells harboring a PTK with inappropriate activity from the effect of the modulator on the difference in the rate of cell growth. The modulator can be identified by the methods of the

invention.

The term "inappropriate activity" refers to a PTK that regulates a step in a signal transduction process at a higher or lower rate than normal cells.

Aberrations in the rate of signal transduction can be caused by alterations in the stimulation of a receptor PTK by a growth factor, alterations in the activity of PTK-specific phosphatase, over-expression of a PTK in a cell, or mutations in the catalytic region of the PTK itself.

The term "signal transduction process" describes the steps in a cascade of events where an extracellular signal is transmitted into an intracellular signal.

The term "PTK-specific phosphatase" describes an enzyme that dephosphorylates a particular PTK and thereby regulates that PTK's activity.

Another aspect of the invention is a method of treating a disease associated with a PTK with inappropriate activity in a cellular organism, where the method comprises the steps of: (a) administering the modulator of PTK function to the organism, where the modulator is in an acceptable pharmaceutical preparation; and (b) activating or inhibiting the PTK function to treat the disease.

The term "organism" relates to any living being comprised of at least one cell. An organism can be as simple as one eukaryotic cell or as complex as a mammal.

The term "administering", in reference to an organism, refers to a method of introducing the compound to the organism. The compound can be administered when the cells or tissues of the organism exist within the

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organism or outside of the organism. Cells existing outside the organism can be maintained or grown in cell culture dishes. For cells harbored within the organism, many techniques exist in the art to administer compounds, including (but not limited to) oral, parenteral, dermal, and injection applications. cells outside of the patient, multiple techniques exist in the art to administer the compounds, including (but not limited to) cell microinjection techniques,

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transformation techniques, and carrier techniques. 10

The term "pharmaceutically acceptable composition" refers to a preparation comprising the modulator of PTK activity. The composition is acceptable if it does not appreciably cause irritations to the organism administered the compound.

Preferred embodiments of the of the invention are that the PTK is a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK-1, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Other preferred embodiments of the invention are that the PTK is a non-receptor PTK selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

The summary of the invention described above is non-limiting and other features and advantages of the invention will be apparent from the following detailed description, and from the claims.

#### BRIEF DESCRIPTION OF THE FIGURES

FIG. 1 provides a ribbon diagram of the structure 30 of FGFR1 showing the side chains of tyrosines Tyr-653

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and Tyr-654 and the  $\alpha$  helical ( $\alpha$ C,  $\alpha$ D,  $\alpha$ E,  $\alpha$ EF,  $\alpha$ F- $\alpha$ I),  $\beta$  strand ( $\beta$ 1- $\beta$ 5,  $\beta$ 7,  $\beta$ 8), nucleotide-binding loop, catalytic loop, activation loop and kinase insert regions of the molecule. The termini are denoted by N and C. The loop between  $\beta$ 2 and  $\beta$ 3 is disordered, indicated by a break in the chain in this region.

FIG. 2 provides a stereo view of a  $C_{\alpha}$  trace of FGFR1 shown in the same orientation as FIG. 1, with every tenth amino acid residue marked with a filled circle and every twentieth amino acid residue labeled with a residue number.

FIG. 3 provides a structure-based sequence alignment of human fibroblast growth factor receptor 1 (FGFR1), human fibroblast growth factor receptor 2 (FGFR2), human fibroblast growth factor receptor 3 (FGFR3), human fibroblast growth factor receptor 4 (FGFR4), a D. malanogaster homolog (DFGFR1), a C. elegans homolog (EGL-15) and insulin receptor tyrosine kinase (IRK).

FIGS. 4A and 4B provide ribbon diagrams of the N-terminal lobes (4A) and C-terminal lobes (4B) of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\beta$  sheets (4A) or  $\alpha$ -helices (4B) of the two proteins have been superimposed.

FIG. 5 illustrates the side-chain positions of the tyrosine autophosphorylation sites of FGFR1 on the backbone representation of FGFR1.

FIGS. 6A and 6B are amino acid sequence alignments of the catalytic domains of PTKs, including receptor and non-receptor type PTKs. FIG. 6A depicts one

representative member from each of the eighteen subfamilies of receptor tyrosine kinases. FIG. 6B



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depicts one representative member from each of the subfamilies of cytoplasmic tyrosine kinases. In FIGS. 6A and 6B highly conserved residues are boxed. The position of the glycine-rich domain, kinase insert, catalytic loop, and activation loop are indicated. The numbering is for human FGF-receptor.

# BRIEF DESCRIPTION OF THE CRYSTALLOGRAPHIC ATOMIC STRUCTURAL COORDINATES

10 The crystallographic structural coordinates are located at the end of the section entitled "Examples" and before the claims. Three sets of coordinates can be found in the Protein Data Bank under accession names 1FGK, 1AGW, and 1FGI. The 1FGK coordinates correspond to those listed in Table 1, the 1AGW coordinates correspond to those listed in Table 4, and the 1FGI coordinates correspond to those listed in Table 3. The 1AGW and 1FGI coordinate sets will be publically available in March 1998.

Table 1 provides the atomic structure coordinates of native FGFR1 crystals of the invention as determined by X-ray crystallography; and

Table 2 provides the atomic structure coordinates of FGFR1:AMP-PCP co-crystals of the invention as determined by X-ray crystallography.

Table 3 lists crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The columns (from left to right) are descriptions of the atoms by number and type, amino acid and number containing the atom, the x coordinate, y

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coordinate, z coordinate, bond connectivity, and temperature factor. All of these parameters are well defined in the art.

Table 4 is a file of crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[4-(4-formylpiperazine-1-yl) benzylidenyl]-2-indolinone. The columns are as described in Table 3.

# DETAILED DESCRIPTION OF THE INVENTION

The present invention is directed to the design and identification of modulators of protein tyrosine kinase function that are PTK subfamily specific, non-hydrolyzable under acidic conditions, and highly bioavailable. The three dimensional structures of a PTK optionally complexed with compounds can facilitate design and identification of modulators of PTK function.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes. Schlessinger and Ullrich, 1992, Neuron 9: 383-391. The PTK family is subdivided into members that are receptors and those that are non-receptors. The PTK receptor family contains multiple subfamilies, one of which is the fibroblast growth factor receptor (FGF-R) PTK which is a molecule implicated in regulating angiogenesis a well as cellular proliferation and differentiation. Givol and Yayon, 1992, FASEB J. 6 (15): 3362-3369.

FGF-R1 can mediates cellular functions by its role in one or more cellular signal transduction processes. Cellular signal transduction processes comprise multiple steps that convert an extracellular signal into an

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intracellular signal.

Receptor PTK mediated signal transduction is initiated by binding a specific extracellular ligand, followed by receptor dimerization, and subsequent autophosphorylation of the receptor PTK. The phosphate groups are binding sites for intracellular signal transduction molecules which leads to the formation of protein complexes at the cell membrane. These complexes facilitate an appropriate cellular effect (e.g., cell division, metabolic effects to the extracellular microenvironment) in response to the ligand that began the cascade of events.

Receptor PTKs function as binding sites for several intracellular proteins. Intracellular PTK binding 15 proteins are divided into two principal groups: (1) those which harbor a catalytic domain; and (2) those which lack such a domain but serve as adapters and associate with catalytically active molecules. Songyang et al., 1993, Cell 72:767-778. SH2 (src homology) 20 domains are common adaptors found in proteins which directly bind to the receptor PTK. SH2 domains are harbored by PTK binding proteins of both groups mentioned above. Fantl et al., 1992, Cell 69:413-423; Songyang et al., 1994, Mol. Cell. Biol. 14:2777-2785); 25 Songyang et al., 1993, Cell 72:767-778; and Koch et al., 1991, Science 252:668-678.

The specificity of the interactions between receptor PTKs and the SH2 domains of their binding proteins is determined by the amino acid residues immediately surrounding the phosphorylated tyrosine residue. Differences in the binding affinities of SH2

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domains is correlated with the observed differences in substrate phosphorylation profiles of downstream molecules in the signal transduction process. Songyang et al., 1993, Cell 72:767-778. These observations suggest that the function of each receptor PTK is determined not only by its pattern of expression and ligand availability but also by the array of downstream signal transduction pathways that are activated by a particular receptor. Thus, PTKs provide a controlling regulatory role in signal transduction processes as a consequence of autophosphorylation.

PTK-mediated signal transduction regulates cell proliferative, differentiation, and metabolic responses in cells. Therefore, inappropriate PTK activity can result in a wide array of disorders and diseases. These disorders, which are described below, may be treated by the modulators of PTK function designed or identified by the methods disclosed herein.

The present invention also relates to crystalline 20 polypeptides corresponding to the catalytic domain of receptor tyrosine kinases. Such tyrosine kinases include receptors of a class that are not covalently cross-linked but are understood to undergo ligandinduced dimerization, as well as cytoplasmic tyrosine kinases. Preferably, the crystalline catalytic domains 25 are of sufficient quality to allow for the determination of a three-dimensional X-ray diffraction structure to a resolution of about 1.5 Å to about 2.5 Å. The invention also relates to methods for preparing and crystallizing the polypeptides. The polypeptides themselves, as well 30 as information derived from their crystal structures can

be used to analyze and modify tyrosine kinase activity as well as to identify compounds that interact with the catalytic domain.

The polypeptides of the invention are designed on 5 the basis of the structure of a region in the cytoplasmic domain of the receptor tyrosine kinase that contains the catalytic domain. By way of illustration, FIG. 6A shows the amino acid sequence alignment of the catalytic domains of eighteen human receptor tyrosine 10 kinases; one representative member from each of the eighteen subfamilies is shown. FIG. 6B shows the alignment for cytoplasmic kinases. The applicants have discovered and determined the boundaries of the domain required for crystallization of the resulting 15 polypeptide. Surprisingly, these boundaries differ from that required for catalytic activity. For example, referring to FIG. 6A, the domain required for catalytic activity is generally believed to span about 7 amino acid residues upstream of the first glycine (FIG. 6A 20 residue number 485) of the N-terminal glycine-rich region through about 10 residues beyond the C-terminal conserved arginine (FIG. 6A, residue number 744). However, the additional sequence upstream of the Nterminal glycine-rich region and downstream of the C-25 terminal conserved arginine can be required for crystallization. In particular, at least about 20 amino acid residues (+/- 5 amino acid residues) upstream of the first glycine (i.e., FIG. 6A, residue number 485) in the conserved glycine-rich region of the catalytic 30 domain, and at least about 17 amino acid residues (+/- 5 amino acid residues) downstream of the conserved

arginine (<u>i.e.</u>, FIG. 6A, residue number 744) located at the C-terminal boundary of the catalytic domain can be required to engineer a polypeptide suitable for crystallization.

5 In those situations where the resulting polypeptide contains cysteine residues that interfere with crystallization (e.g., cysteine residue numbers 488 and 584 in the FGF-R1 sequence shown in FIG. 6A), such cysteine residues can be substituted with an appropriate amino acid that does not readily form covalent bonds 10 with other amino acid residues under crystallization conditions; e.g., by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non- $\beta$ -stranded segment, based on secondary structure  $\mathcal{L}$ 15 assignments, are good candidates for replacement. example, cysteines located in regions corresponding to the glycine-rich-loop, the kinase insert, the juxtamembrane region or the activation loop are prime candidates for replacement. However, substitutions of 20 cysteine residues that are conserved among the kinases (e.g., FIG. 6A at positions 725 and 736) are preferably avoided.

#### I. PTK Associated Diseases

Blood vessel proliferative disorders refer to angiogenic and vasculogenic disorders generally resulting in abnormal proliferation of blood vessels. The formation and spreading of blood vessels play important roles in a variety of physiological processes such as embryonic development, corpus luteum formation, wound healing and organ regeneration. They also play a

pivotal role in cancer development. Other examples of blood vessel proliferation disorders include arthritis, where new capillary blood vessels invade the joint and destroy cartilage, and ocular diseases, like diabetic retinopathy, where new capillaries in the retina invade the vitreous, bleed and cause blindness. Conversely, disorders related to the shrinkage, contraction or closing of blood vessels are implicated in such diseases as restenosis.

10 Fibrotic disorders refer to the abnormal formation of extracellular matrix. Examples of fibrotic disorders include hepatic cirrhosis and mesangial cell proliferative disorders. Hepatic cirrhosis is characterized by the increase in extracellular matrix constituents resulting in the formation of a hepatic scar. Hepatic cirrhosis can cause diseases such as cirrhosis of the liver. An increased extracellular matrix resulting in a hepatic scar can also be caused by viral infection such as hepatitis.

Mesangial cell proliferative disorders refer to disorders brought about by abnormal proliferation of mesangial cells. Mesangial proliferative disorders include various human renal diseases, such as glomerulonephritis, diabetic nephropathy, malignant nephrosclerosis, thrombotic microangiopathy syndromes, transplant rejection, and glomerulopathies. The PDGF-R has been implicated in the maintenance of mesangial cell proliferation. Floege et al., 1993, Kidney International 43:478-548.

PTKs are directly associated with the cell proliferative disorders described above. For example,

some members of the receptor PTK family have been associated with the development of cancer. Some of these receptors, like EGFR (Tuzi et al., 1991, Br. J. Cancer 63:227-233; Torp et al., 1992, APMIS 100:713-

- 719) HER2/neu (Slamon et al., 1992, APMIS 100:713-and PDGF-R (Kumabe et al., 1992, Oncogene 7:627-633) are over-expressed in many tumors and/or persistently activated by autocrine loops. In fact, PTK over-expression (Akbasak and Suner-Akbasak et al., 1992, J.
- Neurol. Sci. 111:119-133; Dickson et al., 1992, J.

  Treatment Res. 61:249-273; Korc et al., 1992, J. Clin.

  Invest. 90:1352-1360) and autocrine loop stimulation
  (Lee and Donoghue, 1992, J. Cell. Biol. 118:1057-1070;
  Korc et al., supra; Akbasak and Suner-Akbasak et al.,
- supra) account for the most common and severe cancers. For example, EGFR is associated with squamous cell carcinoma, astrocytoma, glioblastoma, head and neck cancer, lung cancer and bladder cancer. HER2 is associated with breast, ovarian, gastric, lung, pancreas
- and bladder cancer. PDGF-R is associated with glioblastoma, lung, ovarian, melanoma and prostate cancer. The receptor PTK c-met is generally associated with hepatocarcinogenesis and thus hepatocellular carcinoma. Additionally, c-met is linked to malignant
- tumor formation. More specifically, c-met has been associated with, among other cancers, colorectal, thyroid, pancreatic and gastric carcinoma, leukemia and lymphoma. Additionally, over-expression of the c-met gene has been detected in patients with Hodgkins
- disease, Burkitts disease, and the lymphoma cell line.

  The IGF-I receptor PTK, in addition to being



implicated in nutritional support and in type-II diabetes, is also associated with several types of cancers. For example, IGF-I has been implicated as an autocrine growth stimulator for several tumor types, 5 e.g. human breast cancer carcinoma cells (Arteaga et al., 1989, J. Clin. Invest. 84:1418-1423) and small lung tumor cells (Macauley et al., 1990, Cancer Res. 50:2511-2517). In addition, IGF-I, integrally involved in the normal growth and differentiation of the nervous system, 10 appears to be an autocrine stimulator of human gliomas. Sandberg-Nordqvist et al., 1993, Cancer Res. 53:2475-The importance of the IGF-IR and its modulators in cell proliferation is further supported by the fact that many cell types in culture (fibroblasts, epithelial 15 cells, smooth muscle cells, T-lymphocytes, myeloid cells, chondrocytes, osteoblasts, the stem cells of the bone marrow) are stimulated to grow by IGF-I. Goldring and Goldring, 1991, Eukaryotic Gene Expression 1:301-In a series of recent publications suggest that IGF-IR plays a central role in the mechanisms of 20 transformation and, as such, could be a preferred target for therapeutic interventions for a broad spectrum of human malignancies. Baserga, 1995, Cancer Res. 55:249-252; Baserga, 1994, Cell 79:927-930; Coppola et al., 25 1994, Mol. Cell. Biol. 14:4588-4595.

The association between abnormalities in receptor PTKs and disease are not restricted to cancer, however. For example, receptor PTKs are associated with metabolic diseases like psoriasis, diabetes mellitus, wound healing, inflammation, and neurodegenerative diseases. EGF-R is indicated in corneal and dermal wound healing.

Defects in Insulin-R and IGF-IR are indicated in type-II diabetes mellitus. A more complete correlation between specific receptor PTKs and their therapeutic indications is set forth in Plowman et al., 1994, DN&P 7:334-339.

Non-receptor PTKs, including src, abl, fps, yes, fyn, lyn, lck, blk, hck, fgr, yrk (reviewed by Bolen et al., 1992, FASEB J. 6:3403-3409), are involved in the proliferative and metabolic signal transduction pathways also associated with receptor PTKs. Therefore, the

present invention is also directed towards designing modulators against this class of PTKs. For example, mutated src (v-src) is an oncoprotein (pp60v-src) in chicken. Moreover, its cellular homolog, the proto-oncogene pp60c-src transmits oncogenic signals of many

receptors. For example, over-expression of EGF-R or HER2/neu in tumors leads to the constitutive activation of pp60<sup>c-src</sup>, which is characteristic of the malignant cell but absent in the normal cell. On the other hand, mice deficient for the expression of c-src exhibit an osteopetrotic phaneters.

osteopetrotic phenotype, indicating a key participation of c-src in osteoclast function and a possible involvement in related disorders. Similarly, Zap 70 is implicated in T-cell signaling. Both receptor PTKs and non-receptor PTKs are connected to hyperimmune disorders.

The instant invention is directed in part towards designing modulators of PTK function that could indirectly kill tumors by cutting off their source of sustenance. Normal vasculogenesis and angiogenesis play important roles in a variety of physiological processes such as embryonic development, wound healing, organ

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regeneration and female reproductive processes such as follicle development in the corpus luteum during ovulation and placental growth after pregnancy. Folkman and Shing, 1992, J. Biological Chem. 267:10931-34. However, many diseases are driven by persistent unregulated or inappropriate angiogenesis. For example, in arthritis, new capillary blood vessels invade the joint and destroy the cartilage. In diabetes, new capillaries in the retina invade the vitreous, bleed and cause blindness. Folkman, 1987, in: Congress of Thrombosis and Haemostasis (Verstraete, et. al, eds.), Leuven University Press, Leuven, pp.583-596. Ocular neovascularization is the most common cause of blindness and dominates approximately twenty (20) eye diseases.

Moreover, vasculogenesis and/or angiogenesis can be associated with the growth of malignant solid tumors and metastasis. A tumor must continuously stimulate the growth of new capillary blood vessels for the tumor itself to grow. Furthermore, the new blood vessels embedded in a tumor provide a gateway for tumor cells to enter the circulation and to metastasize to distant sites in the body. Folkman, 1990, J. Natl. Cancer Inst. 82:4-6; Klagsbrunn and Soker, 1993, Current Biology 3:699-702; Folkman, 1991, J. Natl., Cancer Inst. 82:4-6; Weidner et al., 1991, New Engl. J. Med. 324:1-5.

Several polypeptides with in vitro endothelial cell growth promoting activity have been identified. Examples include acidic and basic fibroblastic growth factor ( $\alpha$ FGF,  $\beta$ FGF), vascular endothelial growth factor (VEGF) and placental growth factor. Unlike  $\alpha$ FGF and  $\beta$ FGF, VEGF has recently been reported to be an

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endothelial cell specific mitogen. Ferrara and Henzel, 1989, Biochem. Biophys. Res. Comm. 161:851-858; Vaisman et al., 1990, J. Biol. Chem. 265:19461-19566.

Thus, identifying the specific receptors that bind FGF or VEGF is important for understanding endothelial 5 cell proliferation regulation. Two structurally related receptor PTKs that bind VEGF with high affinity are identified: the flt-1 receptor (Shibuya et al., 1990, Oncogene 5:519-524; De Vries et al., 1992, Science

- 255:989-991) and the KDR/FLK-1 receptor, discussed in 10 the U.S. Patent Application No. 08/193,829. addition, a receptor that binds  $\alpha FGF$  and  $\beta FGF$  is identified. Jaye et al., 1992, Biochem. Biophys. Acta 1135:185-199). Consequently, these receptor PTKs most 15
- likely regulate endothelial cell proliferation. FGFRs play important roles in angiogenesis, wound healing, embryonic development, and malignant transformation. Basilico and Moscatelli, 1992, Adv. Cancer Res. 59:115-165. Four mammalian FGFR (FGFR1-4)
- have been described and additional diversity is 20 generated by alternative RNA splicing within the extracellular domains. Jaye et al., 1992, Biochem. Biophys. Acta 1135:185-199. Like other receptor PTKs, dimerization of FGF receptors is essential for their
- 25 activation. Soluble or cell surface-bound heparin sulfate proteoglycans act in concert with FGF to induce dimerization (Schlessinger et al., 1995, Cell 83:357-360), which leads to autophosphorylation of specific tyrosine residues in the cytoplasmic domain. Mohammadi
- 30 et al., 1996, Mol. Cell Biol. 16:977-989.

Mutations in three human FGF receptor genes, FGFR1,



FGFR2, and FGFR3, have been implicated in a variety of human genetic skeletal disorders. Mutations in FGFR1 and FGFR2 result in the premature fusion of the flat bones of the skull and cause the craniosynostosis syndromes, such as Apert (FGFR2) (Wilkie et al., 1994, 5 Nat. Genet. 8:269-274), Pfeiffer (FGFR1 and FGFR2) (Muenke et al., 1994, Nat. Genet. 8:269-274), Jackson-Weiss (FGFR2) (Jabs et al., 1994, Nat. Genet. 8:275-279) and Crouzon (FGFR2) (Jabs et al., 1994, Nat. 10 Genet. 8:275-279) syndromes. In contrast mutations in FGFR3 are implicated in long bone disorders and cause several clinically related forms of dwarfism including achondroplasia (Shiang et al., 1994, Cell 78:335-342), hypochondroplasia (Bellus et al., 1995, Nat. Genet. 15 10:357-359) and the neonatal lethal thanatophoric dysplasia (Tavormina et al., 1995, Nat. Genet. 9:321-328). It has been shown that these mutations lead to constitutive activation of the tyrosine kinase activity of FGFR3 (Webster et al., 1996, EMBO J. 15:520-527). 20 Furthermore gene-targeting experiments in mice have revealed an essential role for FGFR3 in developmental bone formation (Deng et al., 1996, Cell 84:911-921). Another major role proposed for FGFs in vivo is the induction of angiogenesis (Folkman and Klagsbrun, 1987, 25 Science 236:442). Therefore, inappropriate expression of FGFs or of their receptors or aberrant function of the tyrosine kinase activity could contribute to several human angiogenic pathologies such as diabetic retinopathy, rheumatoid arthritis, atherosclerosis and 30 tumor neovascularization (Klagsbrun and Edelman, 1989,

Arteriosclerosis 9:269). Moreover, FGFs are thought to

be involved in malignant transformation. genes coding for the three FGF homologues int-2, FGF-5 and hst-1/K-fgf were originally isolated as oncogenes.

- Furthermore, the cDNA encoding FGFR1 and FGFR2 are amplified in a population of breast cancers (Adnane et 5 al., 1991, Oncogene 6:659-663). Over-expression of FGF receptors has been also detected in human pancreatic cancers, astrocytomas, salivary gland adenosarcomas, Kaposi sarcomas, ovarian cancers and prostate cancers.
- 10 Evidence, such as the disclosure set forth in copending U.S. Application Serial No. 08/193,829, strongly suggests that VEGF is not only responsible for endothelial cell proliferation, but also is a prime regulator of normal and pathological angiogenesis. See
- generally, Klagsburn and Soker, 1993, Current Biology 15 3:699-702; Houck et al., 1992, J. Biol. Chem. 267:26031-26037. Moreover, it has been shown that KDR/FLK-1 and flt-1 are abundantly expressed in the proliferating endothelial cells of a growing tumor, but 20
- not in the surrounding quiescent endothelial cells. Plate et al., 1992, Nature 359:845-848; Shweiki et al., 1992, Nature 359:843-845.

The invention is directed to designing and identifying modulators of receptor and non-receptor PTKfunctions that could modify the inappropriate activity 25 of a PTK involved with a clinical disorder. rational design and identification of modulators of PTKfunctions can be accomplished by utilizing the structural coordinates that define a PTK three 30 dimensional structure.

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## II. <u>Modulators of PTK functions as Therapeutics for</u> Disease

As a consequence of the disorders discussed above, scientists in the biomedical community are searching for modulators of PTK functions that down-regulate signal transduction pathways associated with inappropriate PTK activity.

In particular, small molecule modulators of PTK functions are sought as some can traverse the cell 10 membrane and do not hydrolyze in acidic environments. Some compounds have already been discovered. For example, bis monocyclic, bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808) 1-cyclopropyl-4-pyridyl-15 quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 A1), seleoindoles and selenides (PCT WO 94/03427), 20 tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although some modulators of PTK function are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the oxindolinone/ thiolindolinone family, however, are specific for the FGF receptor subfamily (U.S. Patent Application Serial No. 08/702,232, filed August 23, 1996, invented by Tang et al., entitled "Indolinone Combinatorial Libraries and Related Products and Methods for the Treatment of

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Disease," Attorney Docket No. 221/187). In addition, compounds of the oxindolinone/thiolindolinone family are non-hydrolyzable in acidic conditions and can be highly bioavailable.

5 The invention provides information regarding the specific interactions between a PTK and compounds of the oxindolinone/thiolindolinone family. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, the PTKs in these structures 10 are not complexed with PTK subfamily specific, hydrolysis resistant, highly bioavailable small molecules. The X-ray crystallography techniques used in the current invention resolve interactions between a PTK and compounds in complex with it at the atomic level, which provides detailed information regarding the 15 orientation of chemical groups defining an effective modulator of PTK function.

## III. Crystalline Tyrosine Kinases

Crystalline PTKs of the invention include native crystals, derivative crystals and co-crystals. The native crystals of the invention generally comprise substantially pure polypeptides corresponding to the tyrosine kinase domain in crystalline form.

It is to be understood that the crystalline tyrosine kinase domains of the invention are not limited to naturally occurring or native tyrosine kinase domains. Indeed, the crystals of the invention include mutants of native tyrosine kinase domains. Mutants of native tyrosine kinase domains are obtained by replacing at least one amino acid residue in a native tyrosine

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kinase domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C-terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native tyrosine kinase domain from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root-mean-square deviation of less than or equal to about  $2\dot{A}$  when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the  $C\alpha$  atoms of the native tyrosine kinase domain are included in the superposition.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the tyrosine kinase domain will depend, in part, on the region of the tyrosine kinase domain where the substitution, addition or deletion occurs. In highly variable regions of the molecule, such as those shown in FIG. 6, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, such as those regions shown in FIG. 6, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are wellknown in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility,

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hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative amino acid substitutions are well known in the art.

For tyrosine kinase domains obtained in whole or in part by chemical synthesis, the selection of amino acids available for substitution or addition is not limited to the genetically encoded amino acids. Indeed, the mutants described herein may contain non-genetically encoded amino acids. Conservative amino acid substitutions for many of the commonly known nongenetically encoded amino acids are well known in the art. Conservative substitutions for other amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or 25 add amino acid residues to a native tyrosine kinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, and for crystallization of the polypeptide. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native tyrosine kinase

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domain will be apparent to those of ordinary skill in the art.

It should be noted that the mutants contemplated herein need not exhibit PTK activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the tyrosine kinase domain but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated tyrosine kinase domain. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold, mercury, etc.

The co-crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc.

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IV. Three Dimensional Structure Determination Using Xray Crystallography

X-ray crystallography is a method of solving the three dimensional structures of molecules. The structure of a molecule is calculated from X-ray diffraction patterns using a crystal as a diffraction grating. Three dimensional structures of protein molecules arise from crystals grown from a concentrated aqueous solution of that protein. The process of X-ray crystallography can include the following steps:

- (a) synthesizing and isolating a polypeptide;
- (b) growing a crystal from an aqueous solution comprising the polypeptide with or without a modulator; and
- (c) collecting X-ray diffraction patterns from the crystals, determining unit cell dimensions and symmetry, determining electron density, fitting the amino acid sequence of the polypeptide to the electron density, and refining the structure.

## Production of Polypeptides

The native and mutated tyrosine kinase domain

polypeptides described herein may be chemically
synthesized in whole or part using techniques that are
well-known in the art (see, e.g., Creighton, 1983).

Alternatively, methods which are well known to those
skilled in the art can be used to construct expression
vectors containing the native or mutated tyrosine kinase
domain polypeptide coding sequence and appropriate

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transcriptional/translational control signals. These methods include in vitro recombinant DNA techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989 and Ausubel et al., 1989.

A variety of host-expression vector systems may be utilized to express the tyrosine kinase domain coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the tyrosine kinase domain coding sequence; yeast transformed with recombinant yeast expression vectors containing the tyrosine kinase domain coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing the tyrosine kinase domain coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus; TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the tyrosine kinase domain coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage  $\lambda$ , plac, ptrp,

ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock 5 promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) may 10 be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when 15 generating cell lines that contain multiple copies of the tyrosine kinase domain DNA, SV40-, BPV- and EBVbased vectors may be used with an appropriate selectable marker.

vectors, various types of cells used, methods of incorporating the vectors into the cells, expression techniques, protein purification and isolation methods, and protein concentration methods are disclosed in detail with respect to the protein PYK-2 in PCT

publication WO 96/18738. This publication is incorporated herein by reference in its entirety, including any drawings. Those skilled in the art will appreciate that such descriptions are applicable to the present invention and can be easily adapted to it.

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#### Crystal Growth

Crystals are grown from an aqueous solution containing the purified and concentrated polypeptide by a variety of techniques. These techniques include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. McPherson, 1982, John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189:1-23; Webber, 1991, Adv. Protein Chem. 41:1-36, incorporated by reference herein in its entirety, including all figures, tables, and drawings.

Generally, the native crystals of the invention are grown by adding precipitants to the concentrated solution of the polypeptide corresponding to the PTK catalytic domain. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

For crystals of the invention, it has been found that hanging drops containing about 2.0  $\mu$ L of tyrosine kinase domain polypeptide (10 mg/mL in 10mM Tris-HCl, pH 8.0, 10 mM NaCl and 2 mM dithiothreitol) and 2.0  $\mu$ L reservoir solution (16% w/v polyethylene glycol MW 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% v/v ethylene glycol or glycerol and 100 mM bis-Tris, pH 6.5) suspended over 0.5 mL reservoir buffer for about 3-4 weeks at 4°C provide crystals suitable for high resolution X-ray structure determination.

Those of ordinary skill in the art will recognize
that the above-described crystallization conditions can
be varied. Such variations may be used alone or in

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combination, and include polypeptide solutions containing polypeptide concentrations between about 1 mg/mL and about 60 mg/mL, Tris-HCl concentrations between about 10 mM and about 200 mM, dithiothreitol concentrations between about 0 mM and about 20 mM, pH ranges between about 5.5 and about 7.5; and reservoir solutions containing polyethylene glycol concentrations between about 10% and about 30% (w/v), polyethylene glycol molecular weights between about 1000 and about 20,000,  $(NH_4)_2SO_4$  concentrations between about 0.1 M and about 0.5 M, ethylene glycol or glycerol concentrations between about 0% and about 20% (v/v), bis-Tris concentrations between about 10 mM and about 200 mM, pH ranges between about 5.5 and about 7.5 and temperature ranges between about 0°C and about 25°C. Other buffer solutions may be used such as HEPES buffer, so long as the desired pH range is maintained.

Derivative crystals of the invention can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. It has been found that soaking a native crystal in a solution containing about 0.1 mM to about 5 mM thimerosal, 4-chloromeruribenzoic acid or KAu(CN)<sub>2</sub> for about 2 hr to about 72 hr provides derivative crystals suitable for use as isomorphous replacements in determining the X-ray crystal structure of the tyrosine kinase domain polypeptide.

Co-crystals of the invention can be obtained by soaking a native crystal in mother liquor containing compound that bind the kinase domain, or described above, or can be obtained by co-crystallizing the kinase

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domain polypeptide in the presence of one or more binding compounds.

For co-crystals of tyrosine kinase domain polypeptide in co-complex with AMP-PCP, it has been found that co-crystallizing the kinase domain polypeptide in the presence of AMP-PCP using the abovedescribed crystallization conditions for obtaining native crystals with a polypeptide solution additionally containing 10 mM AMP-PCP and 20 mM MgCl<sub>2</sub> yields cocrystals suitable for the high resolution structure determination by X-ray crystallography. Of course, those having skill in the art will recognize that the concentrations of AMP-PCP and MgCl<sub>2</sub> in the polypeptide solution can be varied, alone or in combination with the variations described above for native crystals. variations include polypeptide solutions containing AMP-PCP concentrations between 0.1 mM and 50 mM and MqCl, concentrations between 0 mM and 50 mM.

a PTK catalytic domain complexed with a compound can be grown by one of two methods. In the first method, the modulator is added to the aqueous solution containing the polypeptide corresponding to the PTK catalytic domain before the crystal is grown. In the second

method, the modulator is soaked into an already existing crystal of a polypeptide corresponding to a PTK catalytic domain.

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#### Crystalline FGFR

In one illustrative embodiment, the invention provides crystals of FGFR1. The crystals were obtained by the methods provided in the Examples. The FGFR1 crystals, which may be native crystals, derivative crystals or co-crystals, have monoclinic unit cells (i.e., unit cells wherein  $a\neq b\neq c$ ;  $\alpha=\gamma=90^\circ$ ; and  $\beta>90^\circ$ ) and space group symmetry C2. There are two FGFR1 molecules in the asymmetric unit, related by an approximate two-fold axis.

Two forms of crystalline FGFR1 were obtained. In one form (designated "C2-A form"), the unit cell has dimensions of a=208.3 Å, b=57.2 Å, c=65.5 Å and  $\beta$ =107.2°. In another form (designated "C2-B form"), the unit cell has dimensions of a=211.6 Å, b=51.3 Å, c=66.1 Å and  $\beta$ =107.7°.

Three distinct two-fold related FGFR1 dimers are observed in both the C2-A and C2-B forms of the FGFR1 crystal, one non-crystallographically related dimer and 20 two crystallographically related dimers. crystallographically related dimer comprises the two molecules in the asymmetric unit. The residues making up the dimer interface are located in C-terminal lobe. In this dimer, the C-terminal lobes abut with the N-25 terminal lobes distal to one another. The total amount of surface area buried in the surface is about 950  $\mbox{\AA}^2$ . Very few of the interactions in the interface are of a specific nature, e.g., hydrogen-bonding or close packing of hydrophobic residues.

There are two crystallographically-related dimers in the C2 lattice. In the first dimer, the residues

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that constitute the dimer interface are limited to those in the  $\beta$ -sheet of the N-terminal lobe (amino acid residues 477, 479, 498, 506, 508 and 496). The total surface area buried in this interface is about  $670 \text{ Å}^2$ The interactions are rather specific. Three hydrophobic residues which are partially solvent-exposed in the monomer, Val-479, Ile-498 and Val-508, come together with their two-fold-related residues to form a compact hydrophobic plug. This plug is capped on either side by a salt bridge between Arg-477 and Glu-496. In addition, two main-chain hydrogen-bonds connect the β-sheets of the two monomers at the start of \$3 (amino acid residues 506 and 508). The residues in this dimer interface, or their residue character, are generally conserved in the mammalian FGF receptors, but not in the invertebrate homologues.

The other crystallographically-related dimer buries about 1650  ${\rm \AA}^2$  in its interface. In this dimer, the  $\alpha C$  helices of the two monomers are nearly parallel and contact each other at their C-terminal ends. Met-534 and Met-537 are in van der Waals contact with their two-fold-related residues. Other hydrophobic contacts involve Pro-466 with Ile-648 and Pro-469 with Ile-676 and Thr-678. In addition, hydrogen bonds (side-chain to main-chain) are made between Arg-470 and Lys-618 and between His-649 and Glu-464, and there are several water molecules that bridge the two monomers through hydrogen bonding.

In the C2-B form of the crystal, the monomers of this second crystallographically-related dimer are shifted slightly with respect to one another (6°

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rotation), indicating that this interface is somewhat fluid.

In both of the crystallographically-related dimers, the N-termini of the two molecules comprising the dimer point in the same direction and are reasonably close to one another.

#### Determining Unit Cell Dimensions and the Three Dimensional Structure of a Polypeptide or Polypeptide Complex

Once the crystal is grown, it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection 15 device. Collection of X-ray diffraction patterns are well documented by those in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. A beam of X-rays enter the crystal and then diffract from the crystal. An X-ray detection device 20 can be utilized to record the diffraction patterns emanating from the crystal. Although the X-ray detection device on older models of these instruments is a piece of film, modern instruments digitally record Xray diffraction scattering.

Methods for obtaining the three dimensional structure of the crystalline form of a peptide molecule or molecule complex are well known in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. The following are steps in the process of determining the three dimensional structure of a molecule or complex from X-ray diffraction data.

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After the X-ray diffraction patterns are collected from the crystal, the unit cell dimensions and orientation in the crystal can be determined. They can be determined from the spacing between the diffraction emissions as well as the patterns made from these emissions. The unit cell dimensions are characterized in three dimensions in units of Angstroms (one  $\dot{A}=10^{-10}$  meters) and by angles at each vertices. The symmetry of the unit cell in the crystals is also characterized at this stage. The symmetry of the unit cell in the crystal simplifies the complexity of the collected data by identifying repeating patterns. Application of the symmetry and dimensions of the unit cell is described below.

15 Each diffraction pattern emission is characterized as a vector and the data collected at this stage of the method determines the amplitude of each vector. phases of the vectors can be determined using multiple techniques. In one method, heavy atoms can be soaked into a crystal, a method called isomorphous replacement, 20 and the phases of the vectors can be determined by using these heavy atoms as reference points in the X-ray analysis. Otwinowski, 1991, Daresbury, United Kingdom, 80-86. The isomorphous replacement method usually 25 requires more than one heavy atom derivative. another method, the amplitudes and phases of vectors from a crystalline polypeptide with an already determined structure can be applied to the amplitudes of the vectors from a crystalline polypeptide of unknown 30 structure and consequently determine the phases of these vectors. This second method is known as molecular

replacement and the protein structure which is used as a reference must have a closely related structure to the protein of interest. Naraza, 1994, Proteins 11:281-296. Thus, the vector information from a PTK of known structure, such as those reported herein, are useful for the molecular replacement analysis of another PTK with unknown structure

Once the phases of the vectors describing the unit cell of a crystal are determined, the vector amplitudes and phases, unit cell dimensions, and unit cell symmetry 10 can be used as terms in a Fourier transform function. The Fourier transform function calculates the electron density in the unit cell from these measurements. electron density that describes one of the molecules or one of the molecule complexes in the unit cell can be 15 referred to as an electron density map. The amino acid structures of the sequence or the molecular structures of compounds complexed with the crystalline polypeptide may then fit to the electron density using a variety of 20 computer programs. This step of the process is sometimes referred to as model building and can be accomplished by using computer programs such as TOM/FRODO. Jones, 1985, Methods in Enzymology 115:157-

A theoretical electron density map can then be calculated from the amino acid structures fit to the experimentally determined electron density. The theoretical and experimental electron density maps can be compared to one another and the agreement between these two maps can be described by a parameter called an R-factor. A low value for an R-factor describes a high

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degree of overlapping electron density between a theoretical and experimental electron density map.

The R-factor is then minimized by using computer programs that refine the theoretical electron density A computer program such as X-PLOR can be used for model refinement by those skilled in the art. Brünger, 1992, Nature 355:472-475. Refinement may be achieved in an iterative process. A first step can entail altering the conformation of atoms defined in an electron density The conformations of the atoms can be altered by simulating a rise in temperature which will increase the vibrational frequency of the bonds and modify positions of atoms in the structure. At a particular point in the atomic perturbation process, a force field, which typically defines interactions between atoms in terms of allowed bond angles and bond lengths, Van der Waals interactions, hydrogen bonds, ionic interactions, and hydrophobic interactions, can be applied to the system of atoms. Favorable interactions may be described in terms of free energy and the atoms can be moved over many iterations until a free energy minimum is achieved. The refinement process can be iterated until the Rfactor reaches a minimum value.

The three dimensional structure of the molecule or molecule complex is described by atoms that fit the theoretical electron density characterized by a minimum R-value. A file can then be created for the three dimensional structure that defines each atom by coordinates in three dimensions. Examples of such structural coordinate files are defined in Table 1, Table 2, Table 3, and Table 4.

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#### V. Structures of FGFR1

The present invention provides high-resolution three-dimensional structures and atomic structure coordinates of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the examples. The atomic structure coordinates of crystalline FGFR1, obtained from the C2-A form of the crystal to 2.0 Å resolution, are listed in Table 3; the coordinates of crystalline FGFR1:AMP-PCP co-complex, obtained from the C2-A form of the crystal to 2.3 Å resolution are listed in Table 4.

15 Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of FGFR1, whether native crystals, 20 derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 1.5 Å when superimposed, using backbone atoms (N,  $C_{\alpha}$ , C and O), on the structure coordinates listed in Table 3 or Table 4 are considered to be identical with the structure coordinates listed in the Tables when at 25 least about 50% to 100% of the backbone atoms of FGFR1 are included in the superposition.

Referring now to FIG. 1, the overall structure of FGFR1 is bi-lobate. The N-terminal lobe of FGFR1 spans amino acid residues 456-567 (FIG. 3) and comprises a curled  $\beta$ -sheet of five anti-parallel strands ( $\beta$ 1- $\beta$ 5) and

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one  $\alpha$ -helix ( $\alpha$ C). The C-terminal lobe spans amino acid residues 568-765 (FIG. 3) and comprises two  $\beta$ -strands ( $\beta$ 7,  $\beta$ 8) and seven  $\alpha$ -helices ( $\alpha$ D,  $\alpha$ E,  $\alpha$ EF,  $\alpha$ F- $\alpha$ I). The secondary structure nomenclature follows that used for IRK (Hubbard et al., 1994) which in turn is based on the assignments for cAPK (Knighton et al., 1991). FIG. 2 shows a stereo view of a  $C_{\alpha}$  trace of FGFR1 in the same orientation as FIG. 1.

A structure-based sequence alignment of the tyrosine kinase domains of human fibroblast growth factor receptor 1 (human FGFR1; labelled FGFR1), human fibroblast growth factor receptors 2, 3 and 4 (labelled FGFR2, FGFR3 and FGFR4, respectively), a D. melanogaster homologue (labelled DFDFR1), a C elegans homologue (labelled EGL-15) and insulin receptor kinase (labelled IRK), is shown in FIG. 3. The sequence of FGFR1, which is not shown in FIG. 3 is identical to the sequence of FGFR1 except that FGFR1 has the following amino acid substitutions and additions: Cys-488 → Ala, Cys-584 → Ser, Leu-457 → Val and an additional five N-terminal amino acids (Ser-Ala-Ala-Gly-Thr). The secondary structure assignments for FGFR1 and IRK were obtained using the Kabsch and Sander algorithm (Kabsch and Sander, 1983) as implemented in PROCHECK (Laskowski et al., 1993). In the FGF receptor sequences, a period represents sequence identity to FGFR1. In the IRK sequence, residues that are identical to FGFR1 are highlighted. A hyphen denotes an insertion.

The numbers under the EGL-15 sequence represent the fractional solvent accessibility (FSA2) of the residue in the FGFR1 structure. The FSA ratio is the ratio of

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the solvent-accessible surface area of a residue in a Gly-X-Gly tripeptide compared to that in the FGFR1 structure. A value of 0 represents an FSA between 0.00 and 0.09; 1 represents an FSA between 0.10 and 0.19, etc. The higher the value, the more solvent-exposed the residue. An asterisk or pound sign in the FSA line indicates that the residue (asterisk) or side chain (pound sign) is not included in the atom model due to disorder. The numbers below the FSA line are the FSAs for those residues that form part of a dimer interface.

The amino acid residue numbers for FGFR1, and hence FGFR1, and IRK provided in FIG. 3 are used in the discussion that follows. Significant differences in the N-terminal lobe of FGFR1 as compared to IRK are found in the loops between  $\beta$  strands and in  $\alpha C.$  Residues from the end of  $\beta 1$  through the beginning of  $\beta 2$  (amino acid residues 485-490) form the nucleotide-binding loop, named because of its role in ATP coordination. This residue stretch contains the protein kinase-conserved GXGXXG sequence motif, where X is any amino acid. loop is poorly ordered in one FGFR1 molecule in the asymmetric unit and disordered (i.e., not included in the atomic model) in the other FGFR1 molecule in the asymmetric unit. The loop between  $\beta1$  and  $\beta3$  is disordered in both FGFR1 molecules comprising the asymmetric unit.

Referring now to FIG. 4A, which provides a ribbon diagram of the N-terminal lobes of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\beta$ -sheets have been superimposed, it can be seen that in FGFR1  $\alpha C$  is longer by one helical turn than in IRK and is oriented such

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that residues Lys-514 and Glu-531, which are conserved in protein kinases, form a salt bridge (represented by a black line). While not intending to be bound by theory, this salt bridge is believed to be important for proper positioning of the conserved lysine side chain, which coordinates two phosphate oxygens of ATP. The salt bridge is observed in the structures of cAPK (Knighton et al., 1991) and mitogen-activated protein kinase (MAPK) (Zhang et al., 1994).

Referring now to FIG. 4B, which provides a ribbon diagram of the C-terminal lobes of FGFR1 and IRK in which the  $C_{\alpha}$  atoms of the  $\alpha$ -helices have been superimposed, a significant difference is found in the C-terminal helix of FGFR1 when compared to IRK; helix  $\alpha$ I of FGFR1 is longer by seven residues (two helical turns) than its counterpart in IRK. The extended length of  $\alpha$ I is presumably important in the biological functioning of FGF receptors, since the tyrosine autophosphorylation site to which an SH2 domain of PLCy binds is six residues C-terminal to this helix.

The structure of FGFR1 displays an open disposition of the N- and C-terminal lobes. Despite having different sets of lattice contacts, the two FGFR1 molecules in the asymmetric unit have only a 2° difference in relative lobe orientation. It appears as though the stearic interaction between residues in  $\alpha$ C (Glu-531 and Met-534) with Phe-642 and Gly-643 of the protein kinase-conserved DFG sequence at the beginning of the activation loop accounts for the open conformation of FGFR1.

The active site of FGFR1 is characterized by at

least amino acid residues spanning the catalytic loop, activation loop and nucleotide binding loop. Unlike the structure of IRK, in which Tyr-1162 occupies the active site of the molecule, the active sites of both FGFR1 molecules in the asymmetric unit are unoccupied.

The activation loop, which regulates phosphorylation, is characterized by at least resides 640 to 663. Quite surprisingly, while the activation loops of FGFR1 and IRK contain the same number of amino 10 acid residues and share greater than 50% sequence homology, the paths of the polypeptide chains are strikingly dissimilar, diverging at Ala-640 (Gly-1149 in IRK) and reconverging at Val-664 (Val-1173 in IRK). Tyr-653 and Tyr 564 are not bound in the active site. Instead, these residues point away from it. Tyr-653 is 15 in van der Waals contact with several hydrophobic residues (Val-664, Leu-672 and Phe-710) and is hydrogenbonded via its hydroxyl group to a backbone carbonyl oxygen (Leu-672). Tyr-654 is more solvent exposed than 20 Tyr-653, and its only van der Waals contact is with Val-Temperature factor data suggest that the activation loop is relatively mobile and adopts multiple conformations.

The catalytic loop of protein kinases lies between secondary structure elements αE and β7 and contains an invariant aspartic acid residue (Asp-623 in FGFR1) which serves as the catalytic base in the phosphotransfer reaction, abstracting the proton from the hydroxyl group of the substrate tyrosine, serine or threonine. The catalytic loop sequence of FGFR1 comprises at least residues His-621 to Asn-628 (amino acid sequence

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HRDLAARN), and is identical to that for IRK and most receptor and non-receptor PTKs.

In addition to the two tyrosine autophosphorylation sites in the activation loop (Tyr-653 and Tyr-654), there are four other autophosphorylation sites present in the FGFR1 crystals of the invention: one in the juxtamembrane region (Tyr-463), two in the kinase insert (Tyr-583 and Tyr-585) and one in the C-terminal lobe (Tyr-730) (Mohammadi et al., 1996). They exhibit varying degrees of conservation in mammalian FGF receptors: Tyr-463 and Tyr-585 in FGFR1 and 2; Tyr-583 in FGFR1, 2 and 3; and Tyr-730 in FGFR 1, 2, 3 and 4 (FIG. 3).

Referring now to FIG. 5, the positions of the autophosphorylation sites are mapped onto the FGFR1 structure. The juxtamembrane site (Tyr-463) and the residues N-terminal to it are disordered in one of the FGFR1 molecules in the asymmetric unit. In the other molecule in the asymmetric unit Tyr-463 is involved in a lattice contact.

The kinase insert region (the region between helices  $\alpha D$  and  $\alpha E$ ) contains autophosphorylation sites Tyr-583 and Tyr-585 and is disordered in both FGFR1 molecules in the asymmetric unit of the C2-A form of the crystal. In the C2-B form, several lattice contacts partially pin down this region in one of the two FGFR1 molecules in the asymmetric unit, allowing a trace of the polypeptide chain to be made. There is no well-defined secondary structure for these residues. Tyr-730, situated in  $\alpha H$  in the C-terminal lobe, is nearly buried and the side-chain hydroxyl group makes two

hydrogen-bonds. The side chains of neighboring Met-732 and Met-733 are both buried. Therefore, phosphorylation of Tyr-730 would presumably require prior unfolding of  $\alpha H$ .

Aside from Tyr-730, the five other
autophosphorylation sites (including Tyr-653 and Tyr654) are found in relatively mobile segments of the
FGFR1 molecule. While not intending to be bound by
theory, the spatial positions of the autophosphorylation
sites relative to the active site suggest that
autophosphorylation occurs by a trans mechanism between
two kinase domains, supporting the hypothesis that
ligand-induced receptor dimerization is critical for the
initiation of autophosphorylation events.

The structure of crystalline FGFR1:AMP-PCP cocomplex is essentially similar to that observed for
crystalline FGFR1. There are no significant changes in
the structure of FGFR1 induced by AMP-PCP binding. In
particular, binding of AMP-PCP, and by extension ATP,
does not by itself promote lobe closure under the
crystallization conditions used. Furthermore,
complexation did not result in any noticeable changes in
the conformations of the activation and nucleotidebinding loops.

The crystalline FGFR1:AMP-PCP co-complex contains hydrogen bonds that are present between N1 of adenine and the amide nitrogen of Ala-564 and between N6 of adenine and the carbonyl oxygen of Glu-562. The adenine ring is flanked on one side by Leu-484 and Val-492 (N-terminal lobe) and on the other side by Leu-630 (C-terminal lobe). The ribose hydroxyl groups make no

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direct hydrogen bonds with protein atoms. Lys-514 is hydrogen-bonded to oxygens of the  $\beta$ - and  $\gamma$ -phosphates. There is no unambiguous electron density that would indicate the positions of Mg² ions. Generally, AMP-PCP appears to be coordinated rather loosely to unphosphorylated FGFR1, being bound to the "roof" of the cleft rather than being tightly sandwiched between the two kinase lobes.

#### 10 Structural Differences Between FGF-R and IRK

Several features distinguish the FGF-receptor structure from that of the insulin-receptor tyrosine kinase. These distinctions are likely to be important in signaling by FGF-receptors, and other monomeric receptors that are believed to undergo ligand-induced dimerization.

The most significant difference between the structures of FGFR1 and IRK is the conformation of the activation loop. In FGFR1, the activation loop is disposed such that the binding site for substrate peptides is blocked not by an activation loop tyrosine, as in IRK, but by Arg-661 and PTK-invariant Pro-663, while the ATP binding site is accessible. This represents another molecular mechanism by which a receptor PTK may be autoinhibited. The observed autoinhibition in FGFR1 would appear to be weaker than that in IRK because of fewer specific interactions made by residues in the FGFR1 activation loop (manifested in the relatively higher B-values) and the accessibility of the ATP site. One obvious distinction between the insulin and FGF receptor families is that in the former,

receptors are covalently linked heterotetramers  $(\alpha_2\beta_2)$ , whereas in the latter, receptor dimerization is ligand dependent. Receptors whose kinase domains are always in close proximity may require a stronger autoinhibition mechanism than those receptors that associate only upon ligand binding (Taylor et al., 1995). Since most growth factor receptors undergo ligand-dependent dimerization and activation, the FGF receptor autoinhibition mechanism appears to be a more general one.

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### VI. <u>Uses of the Crystals and Atomic Structure</u> Coordinates

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals 15 described herein can be used as a starting material in any of the art-known methods of use for receptor and non-receptor tyrosine kinases. Such methods of use include, for example, identifying molecules that bind to 20 the native or mutated catalytic domain of tyrosine The crystals and structure coordinates are particularly useful for identifying compounds that inhibit receptor and non-receptor tyrosine kinases as an approach towards developing new therapeutic agents (see, 25 e.g., Levitzki and Gazit, 1995).

The structure coordinates described herein can be used as phasing models for determining the crystal structures of additional native or mutated tyrosine kinase domains, as well as the structures of co-crystals of such domains with ligands such as inhibitors, agonists, antagonists, and other molecules. The

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structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated tyrosine kinase domains, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of receptor and non-receptor tyrosine kinases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific FGFR1 exemplary crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of the tyrosine kinase domain of any cytoplasmic tyrosine kinase that undergoes ligand-induced dimerization or receptor tyrosine kinase, including but not limited to the tyrosine kinases of FIG. 6.

VII. Structure Determination for PTKs with Unknown Structure Using Structural Coordinates

Structural coordinates, such as those set forth in Table 1, Table 2, Table 3, and Table 4, can be used to determine the three dimensional structures of PTKs with unknown structure. The methods described below can apply structural coordinates of a polypeptide with known structure to another data set, such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Preferred embodiments of the invention relate to determining the three dimensional structures of PTKs and related polypeptides. These include receptor PTKs such as FGF-

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R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Non-receptor PTKs such as SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK can also be used in the methods described herein.

### Structures Using Amino Acid Homology

Homology modeling is a method of applying structural coordinates of a polypeptide of known structure to the amino acid sequence of a polypeptide of 10 unknown structure. This method is accomplished using a computer representation of the three dimensional structure of a polypeptide or polypeptide complex, the computer representation of amino acid sequences of the polypeptides with known and unknown structures, and 15 standard computer representations of the structures of amino acids. Homology modeling comprises the steps of (a) aligning the amino acid sequences of the polypeptides with and without known structure; (b) 20 transferring the coordinates of the conserved amino acids in the known structure to the corresponding amino acids of the polypeptide of unknown structure; refining the subsequent three dimensional structure; and (d) constructing structures of the rest of the polypeptide. One skilled in the art recognizes that conserved amino 25 acids between two proteins can be determined from the sequence alignment step in step (a).

The above method is well known to those skilled in the art. Greer, 1985, Science 228, 1055. Blundell et al., 1988, Eur. J. Biochem. 172, 513. A computer program currently utilized for homology modeling by

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those skilled in the art is the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc.

Alignment of the amino acid sequence is accomplished by first placing the computer representation of the amino acid sequence of a polypeptide with known structure above the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous (e.g., amino acid side chains that are similar in chemical nature - aliphatic, aromatic, polar, or charged) are grouped together. This method will detect conserved regions of the polypeptides and account for amino acid insertions or deletions.

Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in the computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.

The structures of amino acids located in non-conserved regions are to be assigned manually by either using standard peptide geometries or molecular simulation techniques, such as molecular dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

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The homology modeling method is well known to those skilled in the art and has been practiced using different protein molecules. The three dimensional structure of the polypeptide corresponding to the catalytic domain of a serine/threonine protein kinase, myosin light chain protein kinase, was homology modeled from the cAMP-dependent protein kinase catalytic subunit. Knighton et al., 1992, Science 258:130-135.

### 10 Structures Using Molecular Replacement

Molecular replacement is a method of applying the X-ray diffraction data of a polypeptide of known structure to the X-ray diffraction data of a polypeptide of unknown sequence. This method can be utilized to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. X-PLOR is a commonly utilized computer software package used for molecular replacement. Brünger, 1992, Nature 355:472-475. AMORE is another program used for molecular replacement.

Navaza, 1994, Acta Crystallogr. A50:157-163.

Preferably, the resulting structure does not exhibit a root-mean-square deviation of more than 3 Å.

A goal of molecular replacement is to align the
positions of atoms in the unit cell by matching electron
diffraction data from two crystals. A program such as
X-PLOR can involve four steps. A first step can be to
determine the number of molecules in the unit cell and
define the angles between them. A second step can
involve rotating the diffraction data to define the
orientation of the molecules in the unit cell. A third

step can be to translate the electron density in three dimensions to correctly position the molecules in the unit cell. Once the amplitudes and phases of the X-ray diffraction data is determined, an R-factor can be calculated by comparing electron diffraction maps calculated experimentally from the reference data set and calculated from the new data set. An R-factor between 30-50% indicates that the orientations of the atoms in the unit cell are reasonably determined by this method. A fourth step in the process can be to decrease the R-factor to roughly 20% by refining the new electron density map using iterative refinement techniques described herein and known to those or ordinary skill in the art.

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#### Structures Using NMR Data

Structural coordinates of a polypeptide or polypeptide complex derived from X-ray crystallographic techniques can be applied towards the elucidation of three dimensional structures of polypeptides from nuclear magnetic resonance (NMR) data. This method is used by those skilled in the art. Wuthrich, 1986, John Wiley and Sons, New York: 176-199; Pflugrath et al., 1986, J. Molecular Biology 189:383-386; Kline et al., 1986, J. Molecular Biology 189:377-382. While the secondary structure of a polypeptide is often readily determined by utilizing two-dimensional NMR data, the spatial connections between individual pieces of secondary structure are not as readily determinable. The coordinates defining a three-dimensional structure of a polypeptide derived from X-ray crystallographic

techniques can guide the NMR spectroscopist to an understanding of these spatial interactions between secondary structural elements in a polypeptide of related structure.

5 The knowledge of spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from twodimensional NMR experiments. Additionally, applying the crystallographic coordinates after the determination of secondary structure by NMR techniques only simplifies 10 the assignment of NOEs relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure. Conversely, using the crystallographic coordinates to simplify NOE data while determining secondary structure of the polypeptide would bias the NMR analysis of protein structure.

As the analysis of polypeptide structure by NMR methods is a relatively new technique, the use of structural coordinates defining a PTK structure will most likely be utilized more frequently in the near future. As the method progresses, the three dimensional structure analysis of polypeptides of the same size as a PTK catalytic domain will become more frequent.

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VIII. Structure-Based Design of Modulators of PTK Function Utilizing Structural Coordinates Structure-based modulator design and identification methods are powerful techniques that can involve searches of computer data bases containing a wide variety of potential modulators and chemical functional

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groups. The computerized design and identification of modulators is useful as the computer data bases contain more compounds than the chemical libraries, often by an order of magnitude. For reviews of structure-based drug design and identification see Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; Colman, 1994, Current Opinion in Struc. Biol. 4: 868.

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The three dimensional structure of a polypeptide defined by structural coordinates can be utilized by these design methods. The structural coordinates of Table 1, Table 2, Table 3, and Table 4 can be utilized by this method. In addition, the three dimensional structures of receptor and non-receptor PTKs determined by the homology, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods. Thus, the structures of receptor PTKs, FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK, can be utilized by the methods described herein. The structures of non-receptor PTKs, SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK, can also be utilized by the rational modulator design method.

#### 25 <u>Design by Searching Molecular Data Bases</u>

One method of rational modulator design searches for modulators by docking the computer representation of compounds from a data base of molecules. Publicly available data bases include:

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a) ACD from Molecular Designs Limited

- b) NCI from National Cancer Institute
- c) CCDC from Cambridge Crystallographic Data Center
- d) CAST from Chemical Abstract Service
- e) Derwent from Derwent Information Limited
- 5 f) Maybridge from Maybridge Chemical Company LTD
  - g) Aldrich from Aldrich Chemical Company
  - h) Directory of Natural Products from Chapman & Hall

One such data base (ACD distributed by Molecular Designs
Limited Information Systems) contains, for example,
200,000 compounds that are synthetically derived or are
natural products. Methods available to those skilled in
the art can convert a data set represented in two
dimensions to one represented in three dimensions.

These methods are enabled by such computer programs as CONCORD from Tripos Associates or DB-Converter from Molecular Simulations Limited.

Multiple methods of structure-based modulator design are known to those in the art. Kuntz et al., 1982, J. Mol. Biol. 162: 269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623.

A computer program widely utilized by those skilled in the art of rational modulator design is DOCK from the University of California in San Francisco. The general methods utilized by this computer program and programs like it are described in three applications below. More detailed information regarding some of these techniques can be found in the Molecular Simulations User Guide, 1995.

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A typical computer program used for this purpose can comprise the following steps:

- (a) remove the existing compound from the protein;
- (b) dock the structure of another compound into the active-site using the computer program (such as DOCK) or by interactively moving the compound into the active-site;
- (c) characterize the space between the compound and the active-site atoms;
- (d) search libraries for molecular fragments which (i)can fit into the empty space between the compound and the active-site, and (ii) can be linked to the compound; and
  - (e) link the fragments found above to the compound and evaluate the new modified compound.

Part (c) refers to characterizing the geometry and the complementary interactions formed between the atoms of the active-site and the compounds. A favorable geometric fit is attained when a significant surface area is shared between the compound and active-site atoms without forming unfavorable steric interactions.

One skilled in the art would note that the method can be performed by skipping parts (d) and (e) and screening a data base of many compounds.

Structure-based design and identification of modulators of PTK function can be used in conjunction with assay screening. As large computer data base of compounds (around 10,000 compounds) can be searched in a matter of hours, the computer based method can narrow the compounds tested as potential modulators of PTK function in cellular assays.

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The above descriptions of structure-based modulator design are not all encompassing and other methods are reported in the literature:

- (1) CAVEAT: Bartlett et al.,1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M.; Ley, S.V.; Campbell, M.M. eds.; Royal Society of Chemistry: Cambridge, ppl82-196.
  - (2) FLOG: Miller et al., 1994, J. Comp. Aided Molec. Design 8:153.
- 10 (3) PRO Modulator: Clark et al., 1995, J. Comp. Aided Molec. Design 9:13.
  - (4) MCSS: Miranker and Karplus, 1991, Proteins: Structure, Function, and Genetics 11:29.
  - (5) AUTODOCK: Goodsell and Olson, 1990, Proteins: Structure, Function, and Genetics 8:195.
    - (6) GRID: Goodford, 1985, J. Med. Chem. 28:849.

Design by Modifying Compounds in Complex with PTKs
Another way of identifying compounds as potential

modulators is to modify an existing modulator in the polypeptide active-site. For example, the computer representation of modulators can be modified within the computer representation of a PTK active-site. Detailed instructions for this technique can be found in the

Molecular Simulations User Manual, 1995 in LUDI. The computer representation of the modulator is modified by the deletion of a chemical group or groups or by the addition of a chemical group or groups.

Upon each modification to the compound, the atoms
of the modified compound and active-site can be shifted
in conformation and the distance between the modulator

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and the active-site atoms may be scored along with any complimentary interactions formed between the two molecules. Scoring can be complete when a favorable geometric fit and favorable complementary interactions are attained. Compounds that have favorable scores are potential modulators of PTK function.

## Design by Modifying the Structure of Compounds that Bind PTKs

A third method of structure-based modulator design is to screen compounds designed by a modulator building or modulator searching computer program. Examples of these types of programs can be found in the Molecular Simulations Package, Catalyst. Descriptions for using this program are documented in the Molecular Simulations User Guide (1995). Other computer programs used in this application are ISIS/HOST, ISIS/BASE, ISIS/DRAW) from Molecular Designs Limited and UNITY from Tripos Associates.

These programs can be operated on the structure of a compound that has been removed from the active-site of the three dimensional structure of a compound-PTK complex. Operating the program on such a compound is preferable since it is in a biologically active conformation.

A modulator construction computer program is a computer program that may be used to replace computer representations of chemical groups in a compound complexed with a PTK with groups from a computer data base. A modulator searching computer program is a computer program that may be used to search computer

PCT/US97/14885

representations of compounds from a computer data base that have similar three dimensional structures and similar chemical groups as compound bound to a PTK.

A typical program can operate by using the following general steps:

- (a) map the compounds by chemical features such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites;
- (b) add geometric constraints to the mapped features; and
  - (c) search data bases with the model generated in (b).

Those skilled in the art recognize that for indolinones, the important chemical features include, but are not limited to, a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Those skilled in the art also recognize that not all of the possible chemical features of the compound need be present in the model of (b). One can use any subset of the model to generate different models for data base searches.

### IX. Organic Synthetic Techniques

The versatility of computer-based modulator design and identification lies in the diversity of structures screened by the computer programs. The computer programs can search data bases that contain 200,000 molecules and can modify modulators already complexed with the enzyme with a wide variety of chemical

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functional groups. A consequence of this chemical diversity is that a potential modulator of PTK function may take a chemical form that is not predictable. A wide array of organic synthetic techniques exist in the art to meet the challenge of constructing these potential modulators of PTK function. Many of these organic synthetic methods are described in detail in standard reference sources utilized by those skilled in the art. One example of such a reference is March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill. Thus, the techniques required to synthesize a potential modulator of PTK function identified by computer-based methods are readily available to those skilled in the art of organic chemical synthesis.

### X. <u>Cellular Assays Measuring the Effect of a PTK</u> <u>Modulator in Signal Transduction Pathways</u>

20 Cellular assays can be used to test the activity of a potential modulator of PTK function as well as diagnose a disease associated with inappropriate PTK activity. A potential modulator of PTK function can be tested for activity in vitro by assays that measure the 25 effect of a potential modulator on the autophosphorylation of a particular PTK over-expressed in a cell line. Thus, a modulator that acts as a potent inhibitor of the catalytic domain corresponding to a PTK would decrease the amount of autophosphorylation 30 catalyzed by that PTK. Potential modulators could also be tested for activity in cell growth assays in vitro as well as in animal model assays in vivo.

In vivo assays are also useful for testing the bioactivity of a potential modulator designed by the methods of the invention.

Materials, methods, and experimental data for these assays are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

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# XI. Administration of Modulators of PTK Function as Therapeutics for Disease

Methods of administering compounds to organisms as therapeutics for disease are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

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#### EXAMPLES

The examples below are non-limiting and are merely representative of various aspects and features of the present invention. The examples provide illustrative methods for obtaining crystalline forms of protein kinase polypeptides, methods for determining three dimensional structures of these protein kinase polypeptides, and methods for identifying modulators of protein kinases using the three dimensional structures of the protein kinases.

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### EXAMPLE 1: X-ray Crystallographic Structure Determination of FGFR1

#### Polypeptide Synthesis and Isolation

A recombinant baculovirus was engineered to encode residues 456-765 of human FGFRI. A cleavable N-terminal histidine tag was incorporated to aid in protein purification. Three amino acid substitutions were introduced: Cys-488 to Ala, Cys-584 to Ser and Leu-457 to Val. The two cysteine substitutions were made to prevent the formation of disulfide-linked oligomers, which occurs for the native protein. The substitution Leu-457 to Val introduced a Ncol cloning site near Met-456. The codon for Tyr-766 (TAC) was changed to a stop codon (TAG) and a HindIII-cloning site was generated following this stop codon. These substitutions were introduced into the full length human cDNA of FGFR1 in m13MPI9 by site-directed mutagenesis according to the manufacturer's protocol (Amersham).

The resulting construct was digested with *Ncol* and *HindIII* and was ligated into appropriately digested pBlueBac HistagB (Invitrogen). Transfection of insect cells (Sf9) was performed with the BaculoGold transfection system according to the manufacturer's protocol (Pharmingen). Following identification of positive plaques, the recombinant baculovirus was amplified to high titer (5x10<sup>7</sup> virus particles/ml). Sf9 cells were grown in 175-cm<sup>2</sup> flasks to a density of 2-3x10<sup>7</sup> per flask and infected with recombinant baculovirus with a multiplicity of infection (MOI) of 10.

After 48 hr, cells were harvested by centrifugation

at 3,000g for 35 min at 4°C and then lysed in 25 mM

HEPES (pH 7.5), 150 mM NaCl, 10% glycerol, 1.5 mM MgCl<sub>2</sub>,

1 % Triton X-100, 10 µg/ml aprotonin, 10 µg/ml

leupeptin, and 1 mM phenylmethylsulfonyl fluoride

(PMSF). Lysates were centrifuged in a Sorval RC 5C

(Dupont) for 1 hr at 4°C at 40,000g followed by

ultracentrifugation in an XL-80 (Beckman) at 100,000g

for 1 hr. After centrifugation, the clarified lysate

was passed over a Ni<sup>2+</sup> -chelating column (Pharmacia), and

the bound histidine-tagged fusion protein was eluted

with 100 mM imidazole (pH 7.5). Pooled fractions were

loaded onto a Mono Q anion exchange column (Pharmacia)

and eluted with a NaCl gradient from 0 to 500 mM.

The fractions containing the fusion protein were 15 concentrated in a Centricon-30 (Amicon), and the histidine tag was removed by overnight digestion with enterokinase (Biozyme) at 20°C. The digestion was terminated by the addition of aprotonin, leupeptin, PMSF, TPCK, and bovine pancreatic trypsin inhibitor (BPTI). The cleaved kinase domain was then separated 20 from the histidine tag on a Superose 12 size-exclusion column (Pharmacia). The eluted kinase domain was further purified on a Mono Q column. The purified kinase domain was analyzed by N-terminal sequencing and mass spectrometry. Five amino acids (SAAGT) remained 25 from the histidine tag. The predicted molecular mass was confirmed by mass spectrometry.

#### Crystal Growth

Purified FGFR1 was concentrated to 20-50 mg/ml and exchanged into 10 mM Tris-HCl (pH 8.0), 10 mM NaCl, and

2 mM DTT using a Centricon-30. Crystals were grown at  $4^{\circ}\text{C}$  by vapor diffusion in hanging drops containing 2.0  $\mu\text{l}$  of 10 mg/ml protein solution and 2.0  $\mu\text{l}$  of reservoir solution: 16% polyethylene glycol (PEG) 10000, 0.3 M (NH,),SO,, 5% ethylene glycol, and 100 mM bis-Tris (pH 6.5).

Crystals of native FGFR1 were soaked in 500 ml stabilizing solution [25% PEG 10000, 0.3 M (NH4)<sub>2</sub>SO<sub>4</sub>, 0.1 M Bis-Tris (pH 6.5), 5% ethylene glycol] containing 3
[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone (1-5 mM) or 3-[4-(4-formylpiperazine-1-yl)-benzylidenyl]-2-indolinone (1 mM) at 4°C for 24 to 48 hours. The final soaking concentration of DMSO was between 1 to 5%. The crystals cracked at higher concentrations of DMSO.

Co-crystals of FGFR1 with the inhibitors could also be obtained by vapor diffusion in hanging drops containing 2.0  $\mu$ l of 10 mg/ml protein solution and 2.0  $\mu$ l of reservoir solution containing 1 mM 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone and 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone.

Co-crystals of FGFR1 complexed with AMP-PCP were obtained as described for the creation of native crystals, except that the protein solution additionally contained 10 mM AMP-PCP and 20 mM MgCl<sub>2</sub>.

#### Preparation Of Heavy Atom Derivative Crystals

Heavy atom derivative crystals were obtained by soaking FGFR1 native crystals (C2-A form) in a solution containing ethylmercurithiosalicylic acid (thimerosal),

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KAu(CN)<sub>2</sub> or 4-chloromercuribenzoic acid, as provided in Table 1, infra,, and containing 25% PEG 10000, 0.3M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol or glycerol, and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (Synchrotron) or in a dry nitrogen stream at -175°C (rotating anode).

# Data Collection and Structure Determination

For native crystals and crystals comprising the

nucleotide analog AMP-PCP, data were collected either on
a Rigaku RU-200 rotating anode operated at 50 kV and 100
mA (Cu Kα) and equipped with double-focusing mirrors and
an R-AXIS IIC image plate detector, or at beamline X-4A
at the National Synchrotron Light Source, Brookhaven

National Laboratory. Synchrotron data (λ=1.07Å) were

National Laboratory. Synchrotron data (λ=1.07Å) were collected on Fuji image plates and read with a Fuji scanner. One cryo-cooled crystal was used for each of the data sets. To obtain cryo-cooled crystals, crystals were soaked in a cryo-protectant solution containing 25%

PEG 10000, 0.3 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 5% ethylene glycol or glycerol and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (synchrotron data) or in a dry nitrogen stream at -175°C (rotating anode data). All data were processed using DENZO and

SCALEPACK. Otwinowski, 1993, "Oscillation data reduction program," Proceedings of the CCP4 Study Weekend, Sawyer et al., eds. (Daresbury, United Kingdom: SERC Daresbury Laboratory), 56-62.

For native crystals and crystals comprising the nucleotide analog AMP-PCP, a molecular replacement solution was found initially for the C2-B crystal form

using an IRK search model that consisted of polyalanine with the common side chains for residues 993-1263 (FGFR1 residues 475-754), excluding residues 1094-1105 (kinase insert) and 1153-1170 (activation loop). With AMORE 5 (Navaza, 1994, AmoRe: an automated package for molecular replacement," Acta Crystallogr. A50: 157-163), using 80% of the structure factor amplitudes between 15.0 and 3.5 A, one of the two molecules in the asymmetric unit was located. The correlation coefficient (c.c.) for the 10 correct 1-molecule solution was 0.23 (versus 0.20 for the highest incorrect solution). This molecule was rigid body-refined in X-PLOR (Brünger, 1992, X-PLOR (Version 3.1) Manual (New Haven, Conneticut: The Howeard Hughes Medical Institute and Department of Molecular 15 Biophysics and Biochemistry, Yale Uiversity)), first as one rigid body unit, then as two units each comprising a lobe of the kinase. Rigid body refinement (12.0-3.5 Å, F>30) resulted in a relative rotation of the two lobes of ~10° and an increase of the c.c. from 0.20 to 0.25. The rigid body-refined molecule was then used as a new 20 search model in AMORE, and this time both molecules in the asymmetric unit were located. The c.c. for the correct 2-molecule solution was 0.35 (versus 0.27 for the highest incorrect solution).

Multiple cycles of model building and refinement against 6.0-2.4 Å data resulted in the addition to the model of many of the side chains and some of the missing polypeptide chain. Model building was performed using TOM/FRODO (Jones, 1985, "Diffraction methods for biological macromolecules. Interactive computer graphics: FRODO," Methods in Enzymology 115: 157-171)

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and conjugate-gradient minimization and simulated annealing were performed using X-PLOR. Brünger, supra. At this stage, the R-value was 30% (free R-value of 36%). To help expedite model building and refinement, experimental phases were obtained. Because crystals grown in the presence of ethylene glycol were easier to manipulate than those grown in glycerol, several heavy-atom derivative data sets were collected from C2-A crystals that had been soaked in various heavy atom solutions. The C2-B structure was subsequently refined against 6.0-2.4 Å data to an R-value of 23.8% (free R-value of 30.4%) with r.m.s.d. values of 0.008 Å for bond distances and 1.4° for bond angles

Molecular replacement was used to locate the two 15 FGFR1 molecules (designated FLGK-A and FLGK-B) in the asymmetric unit of the C2-A crystal form. Using AMORE with 80% of structure factor amplitudes between 15.0 and 3.5 Å and the C2-B model, the c.c. for the correct 2molecule solution was 0.62 (versus 0.35 for the highest 20 incorrect solution). Heavy atom positions were determined from difference Fourier maps using the calculated phases from the partial model. Refinement of heavy atom parameters and phase determination were performed with MLPHARE (Otwinowski, 1991, "Maximum likelihood refinement of heavy atom parameters," 25 Isomorphous replacement and anomolous Ssattering, Evans and Leslie eds. (Darsbury, United Kingdom: SERC Daresbury Laboratory), 56-62)). An initial molecular isomorphous replacement (MIR)-phased electron density map was calculated with data between 2.0. and 2.8  $\hbox{\normale}{\rm \AA}$ 30 resolution. This map was improved by solvent

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flattening, histogram matching, and non-crystallographic symmetry (NCS) averaging using DM (Cowtan, 1994, "Protein Crystallography," CCP4 and ESF-EACBM Newsletter (joint) 31: 34-38).

Refinement of the C2-A FGFR1 structure against 6.0-2.0 Å data proceeded by conjugate-gradient minimization and simulated annealing using X-PLOR. Tight NCS restraints were imposed until data to 2.0 Å resolution were included in the refinement, at which point the restraints were lifted. An overall anisotropic B-value was calculated using X-PLOR and applied to the observed structure factors, reducing the R-value by ~3%. molecules whose B-values refined to ≥70 Ų were omitted from the subsequent refinement round. The average Bvalue is 37.5  $\mbox{Å}^2$  for all protein atoms, 35.4  $\mbox{Å}^2$  for protein atoms in FLGK-A,  $39.7 \ {\rm \AA}^2$  for protein atoms in FLGK-B, and 40.2 Å<sup>2</sup> for water molecules. The side chains for Cys-603 in FLGK-A and FLGK-B and for Met-534 in FLGK-B have been modeled in two different conformations. Residues that are not included in the atomic model due to poor supporting electron density are for FLGK-A: 456-463, 486-490, 501-504, 580-591, 763-765; and for FLG-B: 456-460, 501-504, 578-593, 646-651, 657-659, 762-765.

The positions of the two AMP-PCP molecules (one per FGFR1 molecule) were easily identified in  $2F_{\text{obs}(\text{co-complex})}$ -  $F_{\text{calc}(\text{FGPR})}$  difference Fourier maps. The AMP-PCP molecule bound to FLGK-B is less tightly bound and has been modeled with an occupancy of 0.5.

Table A summarizes the X-ray crystallography data

sets of FGFR1 derivative crystals that were used to

determine the structures of crystalline FGFR1 and



100 crystalline FGFR1:AMP-PCP co-complex of the invention.

TABLE 5

5	Data Collection and MIR Phasing Summary							
,		Native	AMP-PCP	Thi-12	Thi-2*	PCMB*	L' A(CD.II)	
	X-ray source	X-41	RU-200	RU-200	RU-200	RU-200	KAu(CN)	
	Resolution limit (Å)	2.0	2.3	2.6	2.8		RU-200	
	Number of sites	-		4		2.8	2.8	
	Conc. (mM)/time (h)				7	2	2	
	R <sub>sym</sub> b(%)	4.8(19.7)°	4 5/22 236	0.1/24	0.1/48	0.2/2	5.0/72	
	Total observations	122569	4.5(23.3)°	5.5	9.8	6.8	6.8	
	Unique reflections		91324	55456	59488	67988	45303	
	Completeness (%)	50771	31997	42820 <sup>d</sup>	35538d	18619	18202	
	Signal (%1>3σ)	97.3(96.3)°	95.5(93.7)°	95.0	96.7	98.0	97.7	
	orginar (761250)	80.7(50.3)°	79.6(51.7)°	69.8	66.8	84.7	77.6	
	R <sub>iso</sub> e(%)	<del></del> -		17.1	. 21.2			
	Phasing power <sup>f</sup>				31.2	15.4	15.2	
	R <sub>cullis</sub> g(%)			1.8	2.0	1.0	0.9	
	Overall FOMh		<del></del>	0.55	0.50	0.81	0.84	
	Overall FOM"				0.60		0.04	

<sup>a</sup>Thi-1, Thi-2; ethylmercurithiosalicylic acid (thimerosal); PCMB: 4-chloromercuribenzoic acid.

<sup>d</sup>I(+h) and I(-h) processed as independent reflections. Anomalous scattering contributions were included.

 $^eR_{iso} = 100 \text{ x } \Sigma_h \text{ [[F_p(h)\pm F_p(h)]-[F_{PH}(h)][/$\Sigma_h$]} F_p(h)], \text{ where } F_p \text{ and } F_{PH} \text{ are the native and derivative } F_p(h) = 100 \text{ m} \text{ for } F_p(h) = 100 \text{ m} \text{ fo$ structure factors, respectively.

Phasing power: r.m.s. heavy atom structure factor / r.m.s. lack of closure (for acentric reflections from 20.0 to 2.8Å).

30  $^{g}R_{cullis} = 100 \times \Sigma_{h} \left| \left| F_{PH}(h) \right| - F_{H(calc)}(h) \left| / \Sigma_{h} \right| F_{PH}(h) \pm F_{p}(h) \right|$  (for centric reflections from 20.0 to 2.8Å). <sup>h</sup>Figure of merit:  $\int P(\phi) \exp(i\phi) d\phi / \int P(\phi) d(\phi)$ , where P is the probability distribution of the phase angle φ.

 $<sup>{}^{</sup>b}R_{sym} = 100 \times \Sigma_{h}\Sigma_{i}|I_{i}(h)-\langle I(h)\rangle|/\Sigma_{h}\Sigma_{i}I_{i}(h)$ 

<sup>&</sup>lt;sup>c</sup>Value in parentheses is for the highest resolution shell.

For crystals comprising FGFR1 and compounds 1 and 2, data were collected on a Rigaku RU-200 rotating anode (Cu Ka) operating at 50 kV and 100 mA and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector. One cryo-cooled crystal was used for each of the data sets. Crystals were soaked in a cryo-protectant [25% PEG 10000, 0.3 M (NH.),SO., 5% ethylene glycol, 100 mM bis-Tris (pH 6.5), and 1 mM: [(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2indolinone (hereafter referred to as compound 1) or 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone (hereafter referred to as compound 2) and flash-cooled in a dry nitrogen stream at -175°C. Data were processed using DENZO and SCALEPACK. Otwinowski, 1993, Proceedings of the CCP4 Study Weekend (Daresbury, United Kingdom: SERC Daresbury Laboratory) pp 56-62.

A summary of the data collection parameters are included in the following Table 6:

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TABLE 6

	Resolution limit (Å)	Observa- tions (N)	Complete- ness (%)	Redundan- cy	R <sub>sym</sub> * (%)	Signal (I> $\sigma$ I)
compound 1	2.5	93535	97.6 (96.1)	2.7	6.8 (23.0)	11.8
compound 2	2.4	94093	99.1 (97.9)	3.3	6.3 (32.2)	11.4

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compound 1 structure: 550 residues, 252 water molecules, 2 compound 1 molecules (4589 atoms) compound 2 structure: 550 residues, 248 water molecules, 2 compound 2 molecules (4646 atoms)

#### 30 Structure Analyses

Atomic superpositions were performed with TOSS



(Hendrickson, 1979). Per residue solvent accessible surface calculations were done with X-PLOR. The surface area buried in a dimer interface was calculated with GRASP (Nicholls et al., 1991) using a probe radius of 1.4 Å. The stereochemical quality of the atomic model was monitored using PROCHECK (Laskowski et al., 1993, PROCHECK: a computer program to check the stereochemical quality of protein structures," J. Appl. Cryst. 26: 283-291). As defined in PROCHECK, 93% of the residues in the model have main-chain torsion angles in the most favored Ramachandran regions. There are no residues in disallowed regions, and three residues in generously allowed regions: Arg-622 in FLGK-A and FLGK-B and Arg-554 in FLGK-A. The overall G-factor score is 0.42.

Table 7 summarizes the X-ray crystallography refinement parameters of the structures of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex of the invention. Table 8 summarizes the X-ray crystallography refinement parameters for the FGFR1/compound complexes.

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TABLE 7

	Refinement Parameters									
	FGFR1: 550 residues, 252 water molecules (4580 etc.)									
5	FGFR1:AMP-PCP: 550 residues, 238 water molecules, 2 AMP-PCP molecules (4638 a  Model d-spacings Reflection P									
	Model	d-spacings	Reflection s	R-value <sup>2</sup>	R.m.s.d.					
		(Å)	(N)	(%)	bonds (Å)	angles (°)	B-values			
	FGFR1:	6.0-2.0	42548	21.2 (26.5)			(Ų)			
	FGFR1:AMP-PCP:	6.0-2.3	26729	21.3 (26.2)°	800.0	1.3	1.6			
	*R-value = 100 7		20729	20.1 (27.5)°	0.009	1.4	1.7			

<sup>a</sup>R-value = 100 x  $\Sigma_h$  ||F<sub>obs</sub>(h)| - |F<sub>calc</sub>(h)|| /  $\Sigma_h$ |F<sub>obs</sub>(h)| for reflections with F<sub>obs</sub>>2 $\sigma$ .

TABLE 8

Model d-spacings (Å) Reflec-Rbonds (Å) angles (°) Btions value' (N) values' (Å<sup>2</sup>)compound 6.0 - 2.442548 19.7 0.008 1.3 1.6  $(27.0)^{k}$ compound 6.0 - 2.526729 20.0 800.0 1.4 1.7  $(28.0)^{k}$ 

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15 For bonded protein atoms.

#### Atomic Structural Coordinates

Tables 1 and 2 provide the atomic structural 20 coordinates of unphosphorylated FGFR1 and unphosphorylated FGFR1:AMP-PCP co-complex, respectively. In the Tables, coordinates for both of the FGFR1 molecules of the dimer comprising the asymmetric unit are provided. The amino acid residue numbers coincide 25 with those used in FIG. 3. In the first FGFR1 molecule of the dimer the residue number is preceded by a 1, i.e., residue number 464 of the first FGFR1 molecule of the dimer is denoted by "1464". Tables 3 and 4 provide the atomic structural coordinates of FGFR1 in complex 30 with indolinone compounds found to inhibit FGFR1 function.

<sup>&</sup>lt;sup>b</sup>For bonded protein atoms.

<sup>&#</sup>x27;Value in parentheses is the free R-value (Brünger, 1993) determined from 5% of the data.

 $<sup>{}^{</sup>a}R_{sym} = 100 \times S_{h}S_{i} |I_{i}(h) - I(h)^{0}| / S_{h}S_{i} |I_{i}(h)$ 

<sup>&</sup>lt;sup>c</sup>Value in parentheses is for the highest resolution shell.

<sup>&</sup>lt;sup>i</sup>R-value = 100 x S<sub>h</sub>  $||F_o(h)| - |F_c(h)|| / S_h |F_o(h)|$ , where  $F_o$  and  $F_c$  are the observed and calculated structure factors, respectively  $(F_o > 2s)$ .

<sup>\*</sup>Value in parentheses is the free R-value determined from 5% of the data.

The following abbreviations are used in the Tables:

"Atom Type" refers to the element whose coordinates are provided. The first letter in the column defines the element.

5 "A.A." refers to amino acid.

" $\underline{X}$ ,  $\underline{Y}$  and  $\underline{Z}$ " provide the Cartesian coordinates of the element.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"OCC" refers to occupancy, and represents the percentage of time the atom type occupies the particular coordinate. OCC values range from 0 to 1, with 1 being 100%

"PRT1" or "PRT2" relate to occupancy, with PRT1

designating the coordinates of the atom when in the first conformation and PRT2 designating the coordinates of the atom when in the second or alternate conformation.

Structural coordinates for FGFR1 may be modified by
mathematical manipulation. Such manipulations include,
but are not limited to, crystallographic permutations of
the raw structure coordinates, fractionalization of the
raw structure coordinates, integer additions or
subtractions to sets of the raw structure coordinates,
inversion of the raw structure coordinates and any
combination of the above.

In addition, the structural coordinates can be slightly modified and still render nearly identical three dimensional structures. Therefore, a measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural

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coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed as identical.

### 5 <u>EXAMPLE 2</u>: <u>Computer-Based Design of Modulators of PTK Function</u>

Potential modulators of PTK function were designed and identified by operating the program Catalyst on the structure of 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The chemical features constraining the search model include a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Approximately 40 compounds were identified as potential modulators of PTK function using this method.

The compounds identified by the method as potential modulators of PTK function were commercially available. These compounds were then tested for their ability to inhibit the FLK PTK in an enzyme linked immunosorbant assay (ELISA). The method of performing this assay is taught in WO 96/40116, entitled "Indolinone Compounds for the Treatment of Disease," published on December 19, 1996, invented by Tang et al., incorporated by reference herein in its entirety, including all figures, drawings, and tables. Flk-1 specific antibodies can be prepared from the following protocol:

1. Prepare a Tresyl-Activated Agarose/Flk-1-D column

30 by incubating 10 ml of Tresyl-Activated Agarose
with 20 mg of purified GST-Flk-1-D fusion protein

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in 100mM sodium bicarbonate (pH 9.6) buffer overnight at 4°C.

- 2. Wash the column once with PBS.
- 3. Block the excess sites on the column with 2  ${\rm M}$ glycine for 2 hours at 4°C.
- Wash the column with PBS. 4.
- 5. Incubate the column with Rabbit anti-Flk-1D production bleed for 2 hours at 4°C.
- 6. Wash the column with PBS.
- 10 Elute antiserum with 100 mM Citric Acid, pH3.0 and 7. neutralize the eluate immediately with 2 M Tris, pH 9.0.
  - Dialyize the eluate against PBS overnight at 40C 8. with 3 changes of buffer (sample to buffer ratio is 1:100).
  - Adjust the dialyized antiserum to 5% glycerol and 9. store at -80°C in small aliquotes.
- The Flk-1 ELISA can include a 2,2-azino-bis(3-20 ethylbenz-thiazoline-6-sulfonic acid (ABTS) solution, which can comprise 100mM citric acid (anhydrous), 250 mM  $\mathrm{Na_2HPO_4}$  (pH 4.0), 0.5 mg/ml ABTS (Sigma catalog no. A-The solution is most appropriately stored in dark at 4°C until ready for use.
- 25 The FLK-1 specific antibodies can also be purchased from Santa Cruz Biotechnology (Catalog No. SC-504).

Four of the forty compounds identified as potential modulators of PTK function were potent modulators of FLK function. These molecules have the following

30 structures:

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The modulators inhibit the FLK protein kinase with the following  $IC_{50}$  values:

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TABLE 9

Compound	FLK kinase	FLK kinase	EGFR	IGF-1R
	IC <sub>50</sub>	IC <sub>so</sub>	IC <sub>50</sub>	1C <sub>50</sub>
	(μM)	(μM)	(μM)	(μM)
·	compounds	compounds		
	tested at 100µM	tested at 20µM		
l l	14.8	14	>100	>100
2	15.7	10.6	>100	>100
3	21.4	16.6	68	30.9
4	22.9	16.4	>100	>100

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The invention illustratively described herein may be practiced in the absence of any element or elements, limitation or limitations which is not specifically disclosed herein. The terms and expressions which have

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been employed are used as terms of description and not of limitation, and there is no intention that in the use of such terms and expressions of excluding any equivalents of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention claimed. Thus, it should be understood that although the present invention has been specifically disclosed by preferred embodiments and optional features, modification and variation of the concepts herein disclosed may be resorted to by those skilled in the art, and that such modifications and variations are considered to be within the scope of this invention as defined by the appended claims.

Those references not previously incorporated herein by reference, including both patent and non-patent references, are expressly incorporated herein by reference for all purposes. Other embodiments are within the following claims.

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#### SEOUENCE LISTING

(1) GENERA	L INFORMATION:
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(i) APPLICANT: SUGEN, INCORPORATED

351 Galveston Drive

Redwood City, CA 94063

(ii) TITLE OF INVENTION: CRYSTAL STRUCTURES OF A

PROTEIN TYROSINE KINASE

(iii) NUMBER OF SEQUENCES: 5

(iv) CORRESPONDENCE ADDRESS:

(A) ADDRESSEE: Lyon & Lyon

(B) STREET: 633 West Fifth Street

Suite 4700

(C) CITY: Los Angeles

(D) STATE: California

(E) COUNTRY: U.S.A.

(F) ZIP: 90071-2066

(v) COMPUTER READABLE FORM:

(A) MEDIUM TYPE: 3.5" Diskette, 1.44 Mb

storage

(B) COMPUTER: IBM Compatible

(C) OPERATING SYSTEM: IBM P.C. DOS 5.0

(D) SOFTWARE: FastSEQ for Windows 2.0

(vi) CURRENT APPLICATION DATA:

(A) APPLICATION NUMBER: To Be Assigned

(B) FILING DATE: Herewith

(C) CLASSIFICATION:

(vii) PRIOR APPLICATION DATA:

(A) APPLICATION NUMBER:

(B) FILING DATE:

# (viii) ATTORNEY/AGENT INFORMATION:

(A) NAME:

Warburg, Richard J.

REGISTRATION NUMBER: (B)

32,327

(C) REFERENCE/DOCKET NUMBER: 227/088-PCT

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(C) TELEX:

67-3510

# (2) INFORMATION FOR SEQ ID NO:1:

# (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH:

310 amino acids

(B) TYPE:

amino acid

(C) STRANDEDNESS:

single

(D) TOPOLOGY:

linear

(ii) MOLECULE TYPE:

protein

(iii) HYPOTHETICAL:

NO

# (xi) SEQUENCE DESCRIPTION: SEQ ID NO:1:

Met Leu Ala Gly Val Ser Glu Tyr Glu Leu Pro Glu Asp Pro Arg Trp

Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys Pro Leu Gly Glu Gly

Cys Phe Gly Gln Val Val Leu Ala Glu Ala Ile Gly Leu Asp Lys Asp 40

Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys Met Leu Lys Ser Asp

Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser Glu Met Glu Met Met

Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn Leu Leu Gly Ala Cys 90

Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu Tyr Ala Ser Lys Gly

Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro Pro Gly Leu Glu Tyr 120

Cys Tyr Asn Pro Ser His Asn Pro Glu Glu Gln Leu Ser Ser Lys Asp

Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly Met Glu Tyr Leu Ala 145 150 155

Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala Arg Asn Val Leu Val 165 170

Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe Gly Leu Ala Arg Asp 180

Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr Asn Gly Arg Leu Pro 200

Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp Arg Ile Tyr Thr His 210 215 220

Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu Trp Glu Ile Phe Thr 230 235

Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val Glu Glu Leu Phe Lys 245 250

Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro Ser Asn Cys Thr Asn 260 265 270

Glu Leu Tyr Met Met Arg Asp Cys Trp His Ala Val Pro Ser Gln 275 280

Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu Asp Arg Ile Val Ala

Leu Thr Ser Asn Gln Glu 305 310

#### (2) INFORMATION FOR SEQ ID NO:2:

### (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH:

315 amino acids

(B) TYPE:

amino acid

(C) STRANDEDNESS: single

(D) TOPOLOGY:

linear

(ii) MOLECULE TYPE:

protein

(iii) HYPOTHETICAL:

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:2:

Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu Tyr Glu Leu Pro

Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys 25



- Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Val Leu Ala Glu Ala Ile 35 40 45
- Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys
  50 55 60
- Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser 65 70 75 80
- Glu Met Glu Met Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn 85 90 95
- Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu 100 105 110
- Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro 115 120 125
- Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn Pro Glu Glu Gln 130 135 140
- Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly
  145 150 155 160
- Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala 165 170 175
- Arg Asn Val Leu Val Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe
  180 185 190
- Gly Leu Ala Arg Asp Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr 195 200 205
- Asn Gly Arg Leu Pro Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp 210 215 220
- Arg Ile Tyr Thr His Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu 225 235 240
- Trp Glu Ile Phe Thr Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val 245 250 255
- . Glu Glu Leu Phe Lys Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro 260 265 270
- Ser Asn Cys Thr Asn Glu Leu Tyr Met Met Met Arg Asp Cys Trp His 275 280 285
- Ala Val Pro Ser Gln Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu 290 295 300
- Asp Arg Ile Val Ala Leu Thr Ser Asn Gln Glu 305 310 315

### (2) INFORMATION FOR SEQ ID NO:3:

#### (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH:

351 amino acids

(B) TYPE:

amino acid

(C) STRANDEDNESS: single

(D) TOPOLOGY:

linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL:

NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:3:

Met Arg Gly Ser His His His His His Gly Met Ala Ser Met Thr

Gly Gly Gln Gln Met Gly Arg Asp Leu Tyr Asp Asp Asp Asp Lys Asp 25

Pro Ser Ser Arg Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu 35 40 45

Tyr Glu Leu Pro Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu

Val Leu Gly Lys Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Leu

Ala Glu Ala Ile Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys 85

Val Ala Val Lys Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser

Asp Leu Ile Ser Glu Met Glu Met Met Lys Met Ile Gly Lys His Lys 115 120

Asn Ile Ile Asn Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr 135

Val Ile Val Glu Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln 150 155

Ala Arg Arg Pro Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn 165 170

Pro Glu Glu Gln Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln 180 185

Val Ala Arg Gly Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg 200

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Asp	210	Ala	a Ala	a Arç	, Asn	Val 215	. Leu	ı Va]	Thi	Gli	220	Ası )	n Val	l Met	Ly:
Ile 225	Ala	Asp	Phe	e Gly	Leu 230	Ala	Arg	Asp	) Ile	His 235	His	; Ile	e Asp	туг	Ty:
Lys	Lys	Thr	Thr	Asn 245	Gly	Arg	Leu	Pro	Val 250	Lys	Trp	Met	Ala	Pro 255	
Ala	Leu	Phe	Asp 260	Arg	Ile	Tyr	Thr	His 265	Gln	Ser	Asp	Val	Trp		Phe
Gly	Val	Leu 275	Leu	Trp	Glu	Ile	Phe 280	Thr	Leu	Gly	Gly	Ser 285		Tyr	Pro
Gly	Val 290	Pro	Val	Glu	Glu	Leu 295	Phe	Lys	Leu	Leu	Lys 300	Glu	Gly	His	Arg
Met 305	Asp	Lys	Pro	Ser	Asn 310	Cys	Thr	Asn	Glu	Leu 315	Tyr	Met	Met	Met	Arg 320
Asp	Cys	Trp	His	Ala 325	Val	Pro	Ser	Gln	Arg 330	Pro	Thr	Phe	Lys	Gln 335	Leu
Val	Glu	Asp	Leu 340	Asp	Arg	Ile	Val	Ala 345	Leu	Thr	Ser	Asn	Gln 350	Glu	

### (2) INFORMATION FOR SEQ ID NO:4:

### (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 933 base pairs (B) TYPE: nucleic acid

(C) STRANDEDNESS: double

(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: cDNA to mRNA

### (xi) SEQUENCE DESCRIPTION: SEQ ID NO:4:

ATGCTAGCAG GGGTCTCTGA GTATGAGCTT CCCGAAGACC CTCGCTGGGA GCTGCCTCGG 60
GACAGACTGG TCTTAGGCAA ACCCCTGGGA GAGGGCTGCT TTGGGCAGGT GGTGTTGGCA 120
GAGGCTATCG GGCTGGACAA GGACAAACCC AACCGTGTGA CCAAAGTGGC TGTGAAGATG 180
TTGAAGTCGG ACGCAACAGA GAAAGACTTG TCAGGACCTGA TCTCAGAAAT GGAGATGATG 240
AAGATGATCG GGAAGCATAA GAATATCATC AACCTGCTGG GGGCCTGCAC GCAGGATGGT 300
CCCTTGTATG TCATCGTGGA GTATGCCTCC AAGGGCAACC TGCGGGAGTA CCTGCAGGCC 360
CGGAGGCCCC CAGGGCTGGA ATACTGCTAC AACCCCAGCC ACCACCCAGC GGAGCAGCTC 420



TCCTCCAAGG ACCTGGTGTC CTGCGCCTAC CAGGTGGCCC GAGGCATGGA GTATCTGGCC 480 TCCAAGAAGT GCATACACCG AGACCTGGCA GCCAGGAATG TCCTGGTGAC AGAGGACAAT 540 GTGATGAAGA TAGCAGACTT TGGCCTCGCA CGGGACATTC ACCACATCGA CTACTATAAA 600 AAGACAACCA ACGGCCGACT GCCTGTGAAG TGGATGGCAC CCGAGGCATT ATTTGACCGG 660 ATCTACACCC ACCAGAGTGA TGTGTGGTCT TTCGGGGTGC TCCTGTGGGA GATCTTCACT 720 CTGGGCGGCT CCCCATACCC CGGTGTGCCT GTGGAGGAAC TTTTCAAGCT GCTGAAGGAG 780 GGTCACCGCA TGGACAAGCC CAGTAACTGC ACCAACGAGC TGTACATGAT GATGCGGGAC 840 TGCTGGCATG CAGTGCCCTC ACAGAGACCC ACCTTCAAGC AGCTGGTGGA AGACCTGGAC 900 CGCATCGTGG CCTTGACCTC CAACCAGGAG TAG 933

#### (2) INFORMATION FOR SEQ ID NO:5:

#### (i) SEQUENCE CHARACTERISTICS:

(A) LENGTH:

1056 base pairs

(B) TYPE:

nucleic acid

(C) STRANDEDNESS: double

(D) TOPOLOGY:

linear

(ii) MOLECULE TYPE:

CDNA

#### (xi) SEQUENCE DESCRIPTION: SEQ ID NO:5:

ATGCGGGGTT CTCATCATCA TCATCATCAT GGTATGGCTA GCATGACTGG TGGACAGCAA 60 ATGGGTCGGG ATCTGTACGA CGATGACGAT AAGGATCCGA GCTCGAGATC TGCAGCTGGT 120 ACCATGGTAG CAGGGGTCTC TGAGTATGAG CTTCCCGAAG ACCCTCGCTG GGAGCTGCCT 180 CGGGACAGAC TGGTCTTAGG CAAACCCCTG GGAGAGGGCG CCTTTGGGCA GGTGGTGTTG 240 GCAGAGGCTA TCGGGCTGGA CAAGGACAAA CCCAACCGTG TGACCAAAGT GGCTGTGAAG 300 ATGTTGAAGT CGGACGCAAC AGAGAAAGAC TTGTCAGACC TGATCTCAGA AATGGAGATG 360 ATGAAGATGA TCGGGGAAGCA TAAGAATATC ATCAACCTGC TGGGGGCCTG CACGCAGGAT 420 GGTCCCTTGT ATGTCATCGT GGAGTATGCC TCCAAGGGCA ACCTGCGGGA GTACCTGCAG 480 GCCCGGAGGC CCCCAGGGCT GGAATACTCC TACAACCCCA GCCACAACCC AGAGGAGCAG 540 CTCTCCTCCA AGGACCTGGT GTCCTGCGCC TACCAGGTGG CCCGAGGCAT GGAGTATCTG 600 GCCTCCAAGA AGTGCATACA CCGAGACCTG GCAGCCAGGA ATGTCCTGGT GACAGAGGAC 660



AATGTGATGA	AGATAGCAGA	CTTTGGCCTC	. CC2 CCC22			
AATGTGATGA		1000010	GCACGGGACA	TTCACCACAT	CGACTACTAT	720
AAAAAGACAA (	CCAACGGCCG	ACTGCCTGTG	AAGTGGATGG	CACCCCA		
CGGATCTACA	7.0.0			CACCCGAGGC	ATTATTTGAC	780
CGGATCTACA (	CCACCAGAG	TGATGTGTGG	TCTTTCGGGG	TGCTCCTGTG	GGAGATIGTTO	
ACTCTGGGCG G	CTCCCCATA	CCCCCCCCC	_		OGAGAICTTC	840
ACTCTGGGCG G		CCCCGGTGTG	CCTGTGGAGG	AACTTTTCAA	GCTGCTGAAG	900
GAGGGTCACC G	CATGGACAA	GCCCAGTAAC	TGCACCAACC	1000		300
GACTCCTCC			TOCACCAACG	AGCTGTACAT	GATGATGCGG	960
GACTGCTGGC A	TGCAGTGCC	CTCACAGAGA	CCCACCTTCA	AGCAGCTGCT	00220	
SACCGCATCG TO	GGCCTTCA C			110011001001	GGAAGACCTG	1020
GACCGCATCG TO	GGCC11GAC (	CTCCAACCAG	GAGTAG			305-
						1056



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### TABLE 1

At-		Atom Type	A.A	A.A No.	x	Y	Z	occ	В	
210		. / pc		110.						
ATOM	1	N	GLU	1464	-13.639	16.975	8.571	1.00	54.29	
ATOM	3	CA	GLU	1464	-12.479	17.105	7.695	1.00	52.62	
ATOM	4	CB	GLU	1464	-11.400	17.974	8.349	1.00	54.64	
ATOM	5	С	GLU	1464	-11.914	15.738	7.319	1.00	49.74	
MOTA	6	Ō	GLU	1464	-11.845	15.407	6.136	1.00	52.04	
ATOM	7	N	LEU	1465	-11.562	14.925	8.310	1.00	44.95	
ATOM	9	CA	LEU	1465	-11.018	13.599	8.037	1.00	41.04	
ATOM	10	СВ	LEU	1465	-10.236	13.066	9.235	1.00	40.18	
ATOM	11	CG	LEU	1465	-8.719	13.196	9.130	1.00	43.70	
ATOM	12	CD1	LEU	1465	-8.346	14.654	8.891	1.00	46.74	
ATOM	13	CD2	LEU	1465	-8.061	12.671	10.395	1.00	40.72	
ATOM	14	C	LEU	1465	-12.092	12.594	7.656	1.00	39.18	
ATOM	15	0	LEU	1465	-13.187	12.590	8.219	1.00	38.05	
ATOM	16	N	PRO	1466	-11.802	11.748	6.657	1.00	37.20	
MOTA	17	CD	PRO	1466	-10.597	11.793	5.810	1.00	36.41	
ATOM	18	CA	PRO	1466	-12.741	10.727	6.189	1.00	36.13	
ATOM	19	CB	PRO	1466	-12.110	10.262	4.878	1.00	37.50	
ATOM	20	CG	PRO	1466	-10.629	10.459	5.135	1.00	36.20	
MOTA	21	С	PRO	1466	-12.846	9.595	7.201	1.00	35.61	
ATOM	22	0	PRO	1466	-11.847	9.174	7.788	1.00	35.18	
ATOM	23	N	GLU	1467	-14.060	9.121	7.429	1.00	35.38	
ATOM	25	CA	GLU	1467	-14.268	8.053	8.377	1.00	35.43	
MOTA	26	CB	GLU	1467	-15.744	7.965	8.746	1.00	41.10	
MOTA	27	CG	GLU	1467	-16.375	9.280	9.098	1.00	48.25	
ATOM	28	CD	GLU	1467	-17.819	9.145	9.596	1.00	50.24	
ATOM	29	OE1	GLU	1467	-18.446	8.071	9.378	1.00	52.82	
ATOM	30	OE2	GLU	1467	-18.314	10.109	10.230	1.00	51.26	
MOTA	31	C	GLU	1467	-13.838	6.714	7.801	1.00	32.65	
ATOM	32	0	GLU	1467	-13.899	6.511	6.591	1.00	35.06	
ATOM	33	N	ASP	1468	-13.299	5.854	8.659	1.00	30.46	
ATOM	35	CA	ASP	1468	-12.883	4.516	8.262	1.00	28.85	
ATOM	36	CB	ASP	1468	-11.384	4.424	7.975	1.00	29.34	
ATOM	37	CG	ASP	1468	-10.985	3.072	7.408	1.00	27.57	
MOTA	38	OD1	ASP	1468	-11.833	2.159	7.359	1.00	27.78	
MOTA	39	OD2	ASP	1468	-9.817	2.916	7.003	1.00	30.64	
ATOM	40	С	ASP	1468	-13.252	3.564	9.384	1.00	29.29	
ATOM	41	0	ASP	1468	-12.481	3.364	10.336	1.00	27.76	
ATOM	42	N	PRO	1469	-14.435	2.939	9.268	1.00	28.99	
MOTA	43	CD ·	PRO	1469	-15.354	3.091	8.120	1.00	28.09	
MOTA	44	CA	PRO	1469	-14.971	1.987	10.244	1.00	30.01	
ATOM	45	CB	PRO	1469	-16.244	1.473	9.553	1.00	33.33	
MOTA	46	CG	PRO	1469	-16.665	2.630	8.690	1.00	30.53	
ATOM	47	С	PRO	1469	-14.012	0.848	10.563	1.00	28.96	
ATOM	48	0	PRO	1469	-14.085	0.251	11.636	1.00	28.52	
ATOM	49	N	ARG	1470	-13.106	0.556	9.631	1.00	27.59	
ATOM	51	CA	ARG	1470	-12.139	-0.520	9.810	1.00	27.37	
ATOM	52	CB	ARG	1470	-11.301	-0.707	8.533	1.00	28.84	

								-					
A	TOM 5	3	CG	ARG 1	470								
A'	TOM 5				470	0	49	-1.2	79 7.	317	1.00	3.0	
A.		_			470			-1.3		068	1.00		
A7	TOM 5				470	-10.4		-0.0		793	1.00		
Α'	FOM 5	_ `			470	-9.6		0.1		823			
	OM 6:	_			470	-9.24		-0.8		999	1.00	32.	
	OM 64	-	_		470	-9.06	57	1.3		686	1.00	33.	
	'OM 6				470	-11.18	30	-0.2			1.00	28.6	
	OM 66				470	-10.75		-1.2			1.00	29.2	
AT			_	RP 14	171	-10.90		0.9			1.00	28.4	
AT		_		'RP 14	171	-9.94		1.3			1.00	27.8	0
ATO		_		'RP 14	71	-8.72		1.94			1.00	28.6	2
ATO		_		RP 14	71	-8.04					1.00	24.9	7
	_			RP 14	71	-7.15		0.97			1.00	24.8	6
AT(		C	E2 T		71	-6.78		-0.06	_		1.00	28.0	
ATC		CI	E3 T	RP 14	71	-6.64		-0.77	-		1.00	29.2	
ATC		CI	)1 T	RP 14		-8.166		-0.46			1.00	26.59	
ATC	. •	NE	El TF	RP 14		-7.413	_	0.86		74 ]	1.00	27.23	
ATO		CZ	22 TF					-0.19		_	.00	30.10	
ATO		CZ	3 TF			-5.912		-1.86		_	.00	28.70	
ATO		CH				-5.778		-1.549			.00	27.18	
ATO		C	TR			-5.424		-2.23		6 1	.00	27.23	
ATO		0	TR			-10.371		2.223			.00	28.42	
ATO	M 82	N	GL			-9.664		2.321	14.44	_	.00	26.48	
ATO		CA				-11.521		2.874	13.29		.00	28.62	
MOTA		CB	GL			-11.981		3.823	14.29			27.16	
ATON		CG	GL	_		-13.245		4.534	13.79			28.89	
ATOM		CD	GL			-13.552		5.869	14.52	_	•	29.09	
ATOM	1 88	OE:		·		-12.692		7.042	14.05			26.43	
ATOM	1 89	OE2		_		-12.134		7.009	12.93	_			
ATOM	90	C	GLU			-12.596		8.024	14.80			28.59	
ATOM	91	ō	GLU			12.217		3.269	15.701			27.28	
ATOM	92	N	LEU			12.763	:	2.196	15.861			25.10	
ATOM		CA	LEU			11.750	:	3.991	16.711			26.48	
ATOM		CB	LEU			11.962	3	3.608	18.104			4.65	
ATOM	96	CG				10.645	3	3.266	18.817			6.27	
ATOM	97	CD1	LEU	•		10.750	3	3.025	20.337			8.24	
ATOM	98	CD2	LEU			11.323		636	20.642			7.23	
ATOM	99	C	LEU			-9.390		.183	21.000	1.0		5.23	
ATOM	100	0	LEU	1473		12.546		.856	18.740			6.33	
ATOM	101	N	LEU	1473	-:	12.122		.973	18.411	1.0		6.52	
ATOM	102	CD	PRO	1474	- :	13.610	4	. 703	19.554	1.0	_	5.16	
ATOM	103		PRO	1474	-:	14.435		. 500	19.770	1.0		8.52	
ATOM	104	CA	PRO	1474	~ ]	14.215		.870	20.207	1.0		9.65	
ATOM	105	CB	PRO	1474		15.368		.251	21.003	1.0		9.18	
ATOM		CG	PRO	1474	- 1	.5.768		.097	20.154	1.0		3.58	
ATOM	106	C	PRO	1474		.3.173		. 528		1.0		3.17	
ATOM	107	0	PRO	1474		2.427		841	21.124	1.0		.75	
ATOM	108	N	ARG	1475	-1	3.107		849	21.828	1.0		.78	
	110	CA	ARG	1475	-1	2.149		588	21.097	1.0	_	.76	
ATOM	111	CB	ARG	1475		2.362			21.900	1.00		.26	
ATOM	112	CG	ARG	1475		2.178		083	21.743	1.00	31	.58	
ATOM	113	CD	ARG	1475		2.048		536	20.342	1.00		.54	
MOTA	114	NE	ARG	1475		2.048 1.733			20.206	1.00		. 96	
ATOM	116	CZ	ARG	1475		0.503	12.		18.813	1.00		.07	
MOTA	117	NH1	ARG	1475			12.		18.352	1.00			
_					- 2	9.470	12.	447	19.186	1.00			
SSSD/55	145. v01												



								040	1.00	34.	54
			ARG	1475	-10	.308	12.669	17.049	1.00	35.	
MOTA	120	NH2	ARG	1475	-12	2.173	8.261	23.371	1.00	37.	
MOTA	123	C	ARG	1475	-13	1.135	8.318	24.036	1.00	36.	68
MOTA	124	0	ASP	1476	-13	3.356	7.958	23.889	1.00	37.	
MOTA	125	N	ASP	1476		3.498	7.647	25.307	1.00	37.	.87
MOTA	127	CA	ASP	1476	-14	4.967	7.759	25.740	1.00	38.	
MOTA	128	CB	ASP	1476	-1	5.851	6.704	25.115	1.00	43.	
MOTA	129	CG	ASP	1476	-1	5.412	6.015	24.179	1.00		.77
MOTA	130	OD1	ASP	1476		7.003	6.558	25.563	1.00		.86
MOTA	131	OD2	ASP	1476		2.922	6.292	25.701	1.00		. 98
MOTA	132	C	ASP	1476	- 1	2.923	5.928	26.878	1.00		.37
MOTA	133	0	ARG	1477		2.478	5.527	24.711	1.00		.84
MOTA	134	N	ARG	1477	_	1.889	4.221	24.961			.84
MOTA	136	CA	ARG	1477	_	12.214	3.262	23.809			.70
MOTA	137	CB	ARG			L3.693	2.965	23.580			.88
MOTA		CG	ARG			14.366	2.365	24.809			3.86
MOTA		CD				14.596	3.372	25.838			1.14
MOTA		NE	ARG			14.845	3.102				0.58
MOTA		CZ				14.906	1.846				3.14
MOTA		NH1				15.024	4.102	27.96			1.30
ATOM		NH2				10.373	4.338	25.10			2.32
MOTA		C	AR( AR(			-9.679	3.362				2.85
MOTA		0				-9.856	5.544	24.97		_	5.64
OTA		N	LE			-8.426	5.739				4.96
ATO		CA	LE	_		-7.964	6.36			_	6.36
ATO!		CB	LE			-6.498	6.29	23.33	1 1.0		30.71
ATO						-6.059	4.83			_	33.97
OTA						-6.335	7.04			_	37.60
OTA		_	2 LE LE			-8.054	6.62				41.20
OTA		_	LE			-8.366	7.81				36.52
OTA		_	V			-7.442	6.02				35.59
OTA		_			79	-7.008	6.74				35.92
OTA				_	79	-7.041	5.82				39.40
OTA				-	79	-6.712	6.62			.00	34.46
TA		-			79	-8.404	5.10			.00	35.36
ATO		_			79	-5.57	7 7.2			.00	32.50
AT	_	_			79	-4.62	2 6.4		• -	.00	37.77
TA	_	_			480	-5.43				.00	42.77
	OM 16				480	-4.13	2 9.0			.00	41.84
	OM 17	-			480	-4.29				.00	42.45
	OM 17				480	-4.99	1 10.3			.00	42.58
	OM 1	. –	-	_	480	-5.13	5 11.7		-	.00	43.09
					480	-4.20	0 9.5		-	.00	45.25
					480	-3.21	11 9.2		-	00	45.47
			_		480	-3.62		739 29.		1.00	46.82
			_		481	-1.9		816 28.		1.00	50.47
		•			1481	-1.0	16 8.			1.00	52.24
					1481	0.2	96 9.	-		1.00	53.41
		. • •	С О		1481	0.3				1.00	53.64
					1482	1.3				1.00	56.19
			N		1482	2.6				1.00	57.19
		184	CA	LYS	1482	3.6	36 8.		.055	1.00	61.02
		185	CB	LYS	1482	5.1	.15 9	. •		1.00	63.12
		186	CG	LYS	1482		_	.831 31	.089	1.00	
1	MOTA	187	CD	٠.							

							120				
	ATOM	188	CE	LYS	1400						
	ATOM	189	NZ	LYS	1482			.547 3	0.395	1 00	
	ATOM	193	C.		1482		52 5		0.899	1.00	
	ATOM	194	ō	LYS	1482		97 9			1.00	
	ATOM	195		LYS	1482	3.29			3.604	1.00	56.56
	N. TTOA	196	N	PRO	1483	3.85			7.791	1.00	55.03
	7.00		CD	PRO	1483	3.85	- •		.323	1.00	58.31
		197	CA	PRO	1483	4.46		191 29	.167	1.00	56.98
		198	CB	PRO	1483	4.91		254 27	.020	1.00	59.52
		199	CG	PRO	1483				.155	1.00	
		200	C	PRO	1483	3.92	- • .	278 28	.141	1.00	58.75
A	TOM 2	01	0	PRO		5.673		335 26	. 834		58.79
A	TOM 2	02			1483	6.509	10.2		731	1.00	61.17
A			~-	LEU	1484	5.728	9.6		700	1.00	61.31
				LEU	1484	6.838	8.7		702	1.00	64.31
					1484	6.349			408	1.00	67.77
				LEU	1484	5.415		-	640	1.00	67.66
		_		LEU	1484	4.943	•	- •	386	1.00	69.00
			CD2 1	LEU :	1484	6.126				1.00	66.76
	FOM 20		C 1		1484		5.9	72 26.		1.00	
	OM 21	.0 (	_		1484	7.934	9.4	31 24.		1.00	67.77
	OM 21	.1 N	_		485	9.117	9.1	15 24.			70.82
	'OM 21	_		_		7.534	10.39		_		71.82
AT	OM 21				485	8.492	11.07	77 22.9			73.28
AT	OM 21	_	_		485	7.819	11.75			1.00	74.53
AT		_	_		485	6.635	12.09			.00	75.19
ATO			_		491	4.406	14.27		22 1		75.61
ATO		_		LN 1	491	4.042		•	38 1		0.72
ATO			B G1	N 1	491	3.033	13.87		94 1		7.33
			GI		191		14.86				6.67
ATC			GI		191	3.486	12.44	9 20.0		_	
ATO		N	VA	'	92	2.581	12.07	19.3			6.66
ATO		CA				4.072	11.650	20.96			5.20
ATO		CB		_	92	3.646	10.274				5.41
ATO	M 226	CG			92	4.680	9.244				3.83
ATO		CG		<del>-</del>	92	4.138	7.849			00 4	1.60
ATO						5.007	9.445			00 43	1.35
ATON		C	VA		92	3.458	10.084				2.72
ATON	-45	0	VAI	14	92	4.335	10.084				.45
ATOM		N	VAI	149	93	2.309	10.437				.86
		CA	VAI			2.029	9.548	23.07	0 1.0		.67
ATOM	_	CB	VAL				9.321	24.47	7 1.0		
ATOM		CG1		_		0.884	10.242	25.013	1.0		.05
ATOM	235	CG2				1.177	11.693	24.722			.64
ATOM	236	C	VAL			0.459	9.844	24.427			. 40
MOTA		O		149		1.626	7.880	24.704			.36
ATOM	238	N	VAL	149		1.129	7.212	23.796			.09
ATOM	240		LEU	149	4	1.927	7.374	25.796		0 39.	.99
ATOM	241	CA	LEU	149		1.535	6.036	25.890	1.0	0 37.	10
ATOM		CB	LEU	149		2.359		26.250	1.0	0 35.	
	242	CG	LEU	1494		2.036	5.542	27.440	1.0	0 35.	
ATOM	243	CD1	LEU	1494			4.161	28.007	1.0		
ATOM	244	CD2	LEU	1494		2.123	3.085	26.931	1.00		
ATOM	245	C	LEU		_	2.998	3.860	29.143		•	90
ATOM	246	ō		1494	-	0.077	6.236	26.648	1.00		
ATOM	247		LEU	1494	-0	.311	7.318		1.00	33.	31
ATOM	249	N	ALA	1495	-0	.740	5.219	27.097	1.00		93
ATOM		CA	ALA	1495		.147		26.435	1.00		35
ATOM	250	CB	ALA	1495	-2		5.292	26.773	1.00	30.6	
AT OF	251	С	ALA	1495			5.937	25.637	1.00		
CCC~ :-					2	. 201	3.893	27.025	1.00		
555D/55	145. v01								- 0	-9.9	,

MOTA	252	0	ALA	1495	-1.944	2.909	26.840	1.00	28.15
ATOM	253	N	GLU	1496	-3.898	3.813	27.488	1.00	30.37
ATOM	255	CA	GLU	1496	-4.537	2.536	27.745	1.00	31.47
ATOM	256	CB	GLU	1496	-4.862	2.392	29.223	1.00	32.48
ATOM	257	CG	GLU	1496	-3.627	2.239	30.093	1.00	37.81
ATOM	258	CD	GLU	1496	-3.938	2.426	31.565	1.00	41.09
ATOM	259	OE1	GLU	1496	-4.328	3.548	31.944	1.00	41.53
ATOM	260	OE2	GLU	1496	-3. <b>7</b> 97	1.453	32.341	1.00	44.12
ATOM	261	C	GLU	1496	-5.806	2.524	26.916	1.00	32.72
ATOM	262	0	GLU	1496	-6.586	3.478	26.954	1.00	33.91
ATOM	263	И	ALA	1497	-5.953	1.494	26.094	1.00	. 31.06
ATOM ATOM	265	CA	ALA	1497	-7.117	1.353	25.239	1.00	32.33
ATOM	266 267	CB	ALA	1497	-6.691	0.879	23.859	1.00	29.56
MOTA	268	C	ALA	1497	-8.056	0.343	25.885	1.00	32.26
ATOM	269	O N	ALA	1497	-7.648	-0.773	26.197	1.00	33.55
ATOM	271	CA	ILE	1498	-9.286	0.759	26.160	1.00	32.99
ATOM	272	CB	ILE	1498	-10.276	-0.126	26.766	1.00	34.00
ATOM	273	CG2	ILE ILE	1498	-11.329	0.668	27.592	1.00	34.69
ATOM	274	CG2	ILE	1498 1498	-12.341 -10.647	-0.288	28.240	1.00	34.24
ATOM	275	CD1	ILE	1498	-10.647	1.496	28.686	1.00	33.56
ATOM	276	C	ILE	1498	-10.994	2.572 -0.830	29.258 25.624	1.00	31.25
ATOM	277	0	ILE	1498	-11.618	-0.181	24.786	1.00	35.71
ATOM	278	N	GLY	1499	-10.890	-2.147	25.573	1.00	34.88 40.43
ATOM	280	CA	GLY	1499	-11.553	-2.884	24.516	1.00	47.63
ATOM	281	C	GLY	1499	-10.670	-3.233	23.330	1.00	53.08
ATOM	282	Ö	GLY	1499	-9.934	-4.226	23.330	1.00	54.97
ATOM	283	N	LEU	1500	-10.713	-2.394	22.294	1.00	54.18
ATOM	285	CA	LEU	1500	-9.957	-2.603	21.055	1.00	55.26
ATOM	286	CB	LEU	1500	-8.444	-2.726	21.305	1.00	55.39
ATOM	287	CG	LEU	1500	-7.562	-1.472	21.241	1.00	54.27
MOTA	288	CD1	LEU	1500	-6.110	-1.891	21.367	1.00	52.89
MOTA	289	CD2	LEU	1500	-7.768	-0.711	19.935	1.00	50.91
MOTA	290	С	LEU	1500	-10.453	-3.830	20.288	1.00	55.39
MOTA	291	0	LEU	1500	-10.376	-4.963	20.774	1.00	56.23
MOTA	292	N	PRO	1505	-13.315	-5.836	25.394	1.00	53.03
ATOM	293	CD	PRO	1505	-13.945	-7.148	25.167	1.00	55.12
MOTA	294	CA	PRO	1505	-14.306	-4.848	25.846	1.00	50.62
ATOM	295	CB	PRO	1505	-15.635	-5.607	25.715	1.00	50.09
MOTA	296	CG	PRO	1505	-15.241	-7.031	25.950	1.00	52.18
MOTA	297	C	PRO	1505	-14.039	-4.348	27.273	1.00	46.35
MOTA	298	0	PRO	1505	-14.065	-3.143	27.524	1.00	45.82
MOTA	299	N	ASN	1506	-13.711	-5.261	28.181	1.00	42.76
MOTA	301	CA	ASN	1506	-13.433	-4.892	29.566	1.00	45.29
MOTA	302	CB	ASN	1506	-14.283	-5.728	30.529	1.00	45.92
MOTA	303	CG	ASN	1506	-15.752	-5.395	30.441	1.00	46.17
ATOM	304	OD1	ASN	1506	-16.132	-4.232	30.390	1.00	48.57
ATOM	305	ND2	ASN	1506	-16.589	-6.418	30.406	1.00	48.63
MOTA	308	C	ASN	1506	-11.954	-5.008	29.939	1.00	45.33
MOTA	309	0	ASN	1506	-11.597	-5.084	31.121	1.00	44.53
MOTA	310	N	ARG	1507	-11.100	-5.010	28.924	1.00	45.63
ATOM	312	CA	ARG	1507	-9.660	-5.122	29.117	1.00	45.57
ATOM	313	CB	ARG	1507	-9.131	-6.354	28.375	1.00	53.33
ATOM	314	CG	ARG	1507	-9.407	-7.685	29.043	1.00	61.39

A	ATOM 3	315	an.								
		316	CD	ARG	1507		6 -8.	028 30	063 ]		
	-	18	NE	ARG	1507	-8.52	5 -9.	٠.	_	1.00	67.74
			CZ	ARG	1507	-7.97		_		.00	74.64
				ARG	1507	-7.16				.00	80.01
		_		ARG	1507	-8.268		-		.00	80.04
	_			ARG	1507	-8.964				.00	83.41
			ο,	ARG	1507	-9.370				.00	40.94
			N 1	/AL	1508	-7.956	_			.00	37.60
			CA 1		1508	-7.190		-		.00	39.33
	OM 33	30 (	CB (		1508					.00	37.26
	OM 33	31 (			1508	-6.854				.00	36.25
	'OM 33	2 (			1508	-8.124	-0.7			00	39.63
	'OM 33	3 0	_		1508	-5.903	-1.7			00	36.92
AT	OM 33					-5.898	-2.8	18 28.1			
AT	OM 33				508	-5.387	-3.85	51 28.6			34.38
ATO	OM 33	_			509	-5.406	-2.14	27.1			32.85
ATO		_	_		509	-4.174	-2.52				30.47
ATO	_	_		_	509	-4.455	-2.95	9 25.02			31.65
ATC					509	-5.426	-4.01	3 25.01	_		34.13
ATC					509	~3.184	-3.45		_		40.74
ATC			TH		509	-3.270	-1.29			_	31.06
ATO		_	TH	IR 1.	509	-3.716	-0.21				28.38
ATO	_		LY	S 1	510	-2.023	-1.44				7.78
ATO				S 19	510	-1.101					9.48
				_	510	0.172	-0.31		5 1.0		0.54
ATO		CG	LY	S 15	10	~0.037	-0.558				7.88
ATO		CD	LY	S 15	10	1.284	-0.600				3.91
ATO		CE	LY		10	1.145	-0.759			0 4	0.30
MOTA		NZ	LY:		10	7.145	-1.674			0 4	6.24
ATON		C	LY			0.338	~1.096	32.187	1.0		9.09
ATOM		0	LYS			-0.757	-0.166		1.00		3.64
ATOM	357	N	VAI			-0.402	-1.142		1.00		3.76
ATOM		CA	IAV			-0.902	1.048	24.856			9.34
ATOM	360	СВ	VAL			-0.627	1.347	23.463			
ATOM	361	CG1				-1.951	1.457	22.658			7.79
ATOM	362	CG2				-2.681	0.111	22.657			1.14
ATOM		C				-2.837	2.561	23.243	1.00		. 56
ATOM		0	VAL			0.123	2.672	23.361			.15
ATOM	365		VAL	151		0.213	3.413	24.338	1.00		. 83
ATOM	367	N	ALA	151		0.705	2.939	22.196	1.00		.14
ATOM	368	CA	ALA	151		1.405	4.192	21.962	1.00		. 86
ATOM		CB	ALA	151	2	2.743	3.935		1.00	25.	. 55
ATOM	369	C	ALA	151	2	0.500	5.009	21.297	1.00	24.	
ATOM	370	О	ALA	151	2 .	-0.061	4.483	21.057	1.00	25.	. 25
	371	N	VAL	151	3	0.340		20.107	1.00	27.	18
ATOM	373	CA	VAL	151		0.520	6.289	21.360	1.00	29.	
ATOM	374	CB	VAL	1513		1.704	7.165	20.573	1.00	32,	
MOTA	375	CG1	VAL	1513			7.713	21.422	1.00	32.	
MOTA	376	CG2	VAL	1513		2.609	8.585	20.574	1.00	32.	
ATOM	377	C	VAL			2.508	6.559	22.031	1.00	32.	
ATOM	378	ō	VAL	1513		0.238	8.334	19.938	1.00	34.	
ATOM	379	N		1513		0.792	9.185	20.635	1.00		
ATOM	381	CA	LYS	1514		0.207	8.367	18.605		34.6	
ATOM	382		LYS	1514		0.859	9.390	17.789	1.00	36.	
ATOM	383	CB	LYS	1514		1.349	8.764	16.489	1.00	36.4	
ATOM	384	CG	LYS	1514		2.250	7.563	16.697	1.00	36.3	
	204	CD	LYS	1514		2.559	6.854		1.00	39.4	
SSSD/55	145 . 0-							15.390	1.00	45.2	9
2220123	143. VU1										



MOTA	385	CE	LYS	1514	3.080	7.815	14.331	1.00	50.70
ATOM	386	NZ	LYS	1514	4.212	8.685	14.798	1.00	51.41
ATOM	390	С	LYS	1514	-0.121	10.496	17.459	1.00	36.75
ATOM	391	0	LYS	1514	-1.228	10.234	16.978	1.00	35.42
MOTA	392	N	MET	1515	0.294	11.731	17.700	1.00	38.12
MOTA	394	CA	MET	1515	-0.545	12.882	17.432	1.00	41.90
MOTA	395	CB	MET	1515	-1.371	13.238	18.668	1.00	43.08
ATOM	396	CG	MET	1515	-0.536	13.601	19.880	1.00	45.01
ATOM	397	SD	MET	1515	-1.561	13.784	21.324	1.00	46.03
ATOM	398	CE	MET	1515	-1.675	12.072	21.885	1.00	44.02
ATOM	399	С	MET	1515	0.314	14.065	17.021	1.00	44.65
ATOM	400	0	MET	1515	1.543	14.013	17.094	1.00	45.64
MOTA	401	N	LEU	1516	-0.347	15.123	16.568	1.00	47.08
ATOM	403	CA	LEU	1516	0.329	16.337	16.134	1.00	48.08
MOTA	. 404	CB	LEU	1516	-0.500	17.033	15.054	1.00	45.50
ATOM	405	CG	LEU	1516	-0.764	16.265	13.764	1.00	43.22
ATOM	406	CD1	LEU	1516	-1.783	17.014	12.946	1.00	40.32
ATOM	407	CD2	LEU	1516	0.540	16.072	12.991	1.00	43.78
ATOM	408	С	LEU	1516	0.516	17.302	17.297	1.00	51.27
ATOM	409	0	LEU	1516	-0.214	17.249	18.291	1.00	50.37
ATOM	410	N	LYS	1517	1.491	18.191	17.157	1.00	55.47
ATOM	412	CA	LYS	1517	1.757	19.207	18.168	1.00	59.10
ATOM	413	СВ	LYS	1517	3.203	19.702	18.068	1.00	61.61
ATOM	414	CG	LYS	1517	4.251	18.669	18.462	1.00	64.82
ATOM	415	CD	LYS	1517	5.635	19.109	18.018	1.00	67.42
ATOM	416	CE	LYS	1517	6.696	18.102	18.432	1.00	71.76
ATOM	417	NZ	LYS	1517	8.021	18.411	17.812	1.00	73.57
ATOM ATOM	421	C	LYS	1517	0.794	20.365	17.920	1.00	59.91
ATOM	422	0	LYS	1517	0.187	20.456	16.852	1.00	59.88
ATOM	423 425	N CA	SER	1518	0.686	21.267	18.886	1.00	61.85
ATOM	426	CB	SER SER	1518 1518	-0.216	22.409	18.760	1.00	63.70
ATOM	427	C	SER	1518	-0.158 0.079	23.274	20.024	1.00	64.21
ATOM	428	0	SER	1518	-0.841	23.263	17.529	1.00	64.37
ATOM	429	и	ASP	1519	1.359	23.757 23.410	16.875 17.202	1.00	66.16
ATOM	431	CA	ASP	1519	1.767	24.217	16.054	1.00 1.00	64.15 64.55
ATOM	432	CB	ASP	1519	3.109	24.217	16.343	1.00	65.84
ATOM	433	C	ASP	1519	1.858	23.441	14.742	1.00	63.95
MOTA	434	0	ASP	1519	2.432	23.931	13.769	1.00	64.95
ATOM	435	N	ALA	1520	1.303	22.232	14.719	1.00	62.57
ATOM	437	CA	ALA	1520	1.329	21.398	13.521	1.00	60.34
ATOM	438	CB	ALA	1520	0.704	20.039	13.810	1.00	60.53
ATOM	439	С	ALA	1520	0.616	22.062	12.353	1.00	58.21
ATOM	440	0	ALA	1520	-0.464	22.631	12.506	1.00	58.32
ATOM	441	N	THR	1521	1.241	22.001	11.186	1.00	55.96
ATOM	443	CA	THR	1521	0.673	22.582	9.981	1.00	54.98
MOTA	444	CB	THR	1521	1.783	23.013	9.031	1.00	53.84
ATOM	445	OG1	THR	1521	2.554	21.862	8.659	1.00	55.84
ATOM	447	CG2	THR	1521	2.693	24.026	9.703	1.00	55.01
ATOM	448	C	THR	1521	-0.184	21.545	9.261	1.00	54.25
ATOM	449	0	THR	1521	-0.190	20.371	9.629	1.00	54.74
ATOM	450	N	GLU	1522	-0.877	21.974	8.212	1.00	53.32
ATOM	452	CA	GLU	1522	-1.702	21.066	7.423	1.00	52.64
ATOM	453	CB	GLU	1522	-2.472	21.829	6.339	1.00	53.55
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ATC ATC			GL		-0.793	20.012	6.78	0 1.00	51.95
ATC			GL		-1.226				
ATC		-	LY		0.464				
ATO							5.96		
ATO					2.730	20.201			
ATO					3.889				
ATO			LY:		3.487	18.388			
ATO.		CE	LYS	_	4.688	17.635			
ATO		NZ	LYS		4.271	16.629			
		C	LYS		1.699	18.391			
ATO		0	LYS		1.747	17.202	6.697		
ATO		N	ASF		1.857	18.828	8.249		
IOTA IOTA		CA	ASF		2.114	17.915	9.351		42.71 42.11
		CB	ASF		2.313	18.701	10.653		44.94
NOTA NOTA		CG	ASP		3.623	19.490	10.673	1.00	
		OD1			3.692	20.512	11.392	1.00	48.90
MOTA		OD2			4.590	19.084	9.990	1.00	51.88
ATOM		С	ASP		0.956	16.931	9.481	1.00	50.06
ATOM		О	ASP	1524	1.164	15.738	9.748	1.00	39.85
ATOM		N	LEU	1525	-0.261	17.438	9.296	1.00	39.01
ATOM		CA	LEU	1525	-1.461	16.610	9.355	1.00	38.32
ATOM		CB	LEU	1525	-2.720	17.470	9.200	1.00	36.16
ATOM		CG	LEU	1525	-4.081		9.186	1.00	35.13
ATOM		CD1	LEU	1525	-4.184	15.668	10.252	1.00	34.70
ATOM		CD2	LEU	1525	-5.162	17.789	9.395	1.00	36.15
ATOM		С	LEU	1525	-1.406	15.560	8.254		32.96
ATOM		0	LEU	1525	-1.575	14.377	8.518	1.00	34.31
ATOM		N	SER	1526	-1.136	16.005	7.030	1.00	33.34
ATOM	489	CA	SER	1526	-1.039	15.128	5.865	1.00	36.40
ATOM	490	CB	SER	1526	-0.669	15.931	4.618	1.00	37.16
MOTA	491	OG	SER	1526	-1.736	16.779	4.245	1.00	38.84
ATOM	493	C	SER	1526	-0.021	14.016	6.044	1.00	49.61
ATOM	494	0	SER	1526	-0.273	12.873	5.670	1.00	35.90
ATOM	495	N	ASP	1527	1.142	14.349	6.591	1.00	36.68
MOTA	497	CA	ASP	1527	2.177	13.342	6.796	1.00	35.89 35.25
ATOM ATOM	498	CB	ASP	1527	3.497	13.998	7.201	1.00	
ATOM	499	CG	ASP	1527	4.100	14.850	6.081	1.00	35.58 37.19
ATOM	500	OD1	ASP	1527	3.750	14.653	4.895	1.00	37.19
ATOM	501	OD2	ASP	1527	4.932	15.726	6.395	1.00	42.93
ATOM	502	C	ASP	1527	1.749	12.274	7.799	1.00	31.77
ATOM	503	0	ASP	1527	2.000	11.090	7.594	1.00	30.58
	504	N	LEU	1528	1.055	12.684	8.853	1.00	31.80
ATOM ATOM	506	CA	LEU	1528	0.581	11.730	9.857	1.00	33.53
	507	CB	LEU	1528	-0.002	12.471	11.076	1.00	
ATOM	508	CG	LEU	1528	-0.440		12.275		32.20
ATOM	509	CD1	LEU	1528	0.705		12.709		32.63
ATOM	510	CD2	LEU	1528	-0.891		13.426		33.09
ATOM	511	C	LEU	1528	-0.468	10.792	9.235		31.52
ATOM	512	0	LEU	1528	-0.494	9.589	9.521		32.89
ATOM	513	N	ILE	1529	-1.336	11.357			32.39
ATOM	515	CA	ILE	1529	-2.376	10.591			33.72
ATOM	516	CB	ILE	1529	-3.336	11.505	_		30.48
ATOM	517	CG2	ILE	1529	-4.229	10.662	_		28.85
MOTA	518	CG1	ILE	1529	-4.200	12.344			28.54
CCCD/FF						~~.037	7.043	1.00	29.52



ATOM	519	CD1	ILE	1529	-5.143	13.308	7.133	1.00	32.07
MOTA	520	C	ILE	1529	-1.698	9.608	6.768	1.00	31.50
MOTA	521	• 0	ILE	1529	-2.009	8.419	6.780	1.00	30.75
ATOM	522	N	SER	1530	-0.749	10.100	5.974	1.00	33.28
ATOM	524	CA	SER	1530	-0.011	9.250	5.038	1.00	32.48
MOTA	525	CB	SER	1530	1.114	10.042	4.368	1.00	37.20
MOTA	526	OG	SER	1530	0.604	11.218	3.766	1.00	49.93
MOTA	528	С	SER	1530	0.583	8.045	5.756	1.00	29.05
MOTA	529	0	SER	1530	0.397	6.909	5.316	1.00	28.66
ATOM	530	N	GLU	1531	1.259	8.290	6.878	1.00	28.21
MOTA	532	CA	GLU	1531	1.880	7.207	7.631	1.00	27.30
ATOM	533	CB	GLU	1531	2.656	7.733	8.839	1.00	28.90
ATOM	534	CG	GLU	1531	3.271	6.609	9.672	1.00	27.17
ATOM	535	CD	GLU	1531	4.047	7.081	10.886	1.00	30.07
MOTA	536	OE1	GLU	1531	4.779	6.244	11.448	1.00	34.78
MOTA	537	OE2	GLU	1531	3.931	8.256	11.291	1.00	31.96
ATOM	538	С	GLU	1531	0.870	6.162	8.072	1.00	27.73
MOTA	539	0	GLU	1531	1.160	4.961	8.028	1.00	28.72
ATOM	540	N	MET	1532	-0.286	6.621	8.555	1.00	29.78
MOTA	542	CA	MET	1532	-1.373	5.734	8.990	1.00	28.79
ATOM	543	CB	MET .	1532	-2.501	6.553	9.646	1.00	28.90
ATOM	544	CG	MET	1532	-3.763	5.741	9.993	1.00	29.73
MOTA	545	SD	MET	1532	-5.089	6.693	10.765	1.00	30.19
ATOM	546	CE	MET	1532	-5.455	7.870	9.494	1.00	26.70
MOTA	547	C	MET	1532	-1.935	4.937	7.796	1.00	28.34
ATOM	548	0	MET	1532	-2.166	3.730	7.893	1.00	26.62
ATOM	549	И	GLU	1533	-2.165	5.624	6.678	1.00	28.85
MOTA	551	CA	GLU	1533	-2.684	4.984	5.467	1.00	28.24
MOTA	552	CB	GLU	1533	-2.936	6.027	4.384	1.00	25.42
ATOM	553	CG	GLU	1533	-4.099	6.956	4.719	1.00	30.05
MOTA	554	CD	GLU	1533	-5.393	6.201	5.021	1.00	29.47
ATOM	555	OE1	GLU	1533	-5.794	5.336	4.211	1.00	29.01
MOTA	556	OE2	GLU	1533	-6.011	6.472	6.073	1.00	33.98
ATOM	557	C	GLU	1533	-1.694	3.944	4.968	1.00	28.01
ATOM	558	0	GLU	1533	-2.072	2.845	4.573	1.00	27.39
ATOM	559	N	MET	1534	-0.416	4.293	5.036	1.00	29.06
ATOM	561	CA	MET	1534	0.662	3.413	4.621	1.00	29.74
ATOM	562	CB	MET	1534	1.992	4.155	4.755	1.00	33.16
MOTA	563	CG	MET	1534	3.198	3.270	4.682	1.00	42.88
ATOM	564	SD	MET	1534	3.805	3.127	3.042	1.00	50.20
ATOM	565	CE	MET	1534	5.137	4.169	3.159	1.00	42.64
ATOM	566	C	MET	1534	0.641	2.156	5.493	1.00	26.90
ATOM	567	0	MET	1534	0.755	1.038	4.990	1.00	27.05
ATOM	568	N	MET	1535	0.512	2.348	6.803	1.00	25.42
MOTA	570	CA	MET	1535	0.437	1.233	7.737	1.00	25.88
MOTA	571	CB	MET	1535	0.325	1.741	9.181	1.00	27.63
ATOM	572	CG	MET	1535	1.607	2.391	9.737	1.00	27.26
MOTA	573	SD	MET	1535	1.584	2.561	11.564	1.00	29.49
ATOM	574	CE	MET	1535	1.294	4.255	11.699	1.00	28.22
MOTA	575	С	MET	1535	-0.754	0.324	7.396	1.00	26.28
MOTA	576	0	MET	1535	-0.645	-0.908	7.469	1.00	25.93
ATOM	577	N	LYS	1536	-1.890	0.928	7.032	1.00	27.19
ATOM	579	CA	LYS	1536	-3.087	0.162	6.647	1.00	27.20
MOTA	580	CB	LYS	1536	-4.257	1.088	6.310	1.00	25.29

							1	26						
	ATOM	581	CG	LYS	152									
	ATOM	582	CD	LYS	1536		897	1.	770	7.49	1 1	0.0	_	
1	MOTA	583	CE		1536		884		820	7.01		.00	23.1	
1	MOTA	584	NZ	LYS	1536	٠.			588	8.17		.00	22.	
7	<b>~</b> ~ .	588	C	LYS	1536		484		541		_	.00	22.2	25
	ma	589		LYS	1536	-2.			699	7.71		.00	23.4	0
			0	LYS	1536	~3.0	069			5.423		. 00	24.5	
		590	N	MET	1537	-2.1	183	-1.		5.403		.00	26.6	
	_	592	CA	MET	1537	-1.8	242	-0.0		4.411		00	27.1	
		593	CB	MET	1537	-1.0	43	-0.8		3.194		00	28.0	
		94	CG	MET	1537	-1.2	69	0.1	47	2.147		00		
	TOM 5	95	~~	MET		-2.2	65	1.1	64	1.591		00	30.3	
A:	rom 5	96	~~	MET	1537	9.0		0.4		0.727			36.3	
	rom 5	97	_	MET	1537	-2.9		-0.0		0.793	1.		42.19	€
AT	COM 5				1537	-0.8		-1.9			1.		36.22	
				/ET	1537	-1.00	50	-3.0	-	3.447	1.6		26.98	}
				LE	1538	0.18		-1.6	~ ~	2.963	1.0	00	25.34	
				LE	1538	1.23		-2.6		.229	1.0		27.69	
				LE	1538	2.45		-2.6		.535	1.0		25.39	
			CG2 I	LE	1538	3.42		-2.00	06 5	.255	1.0		24.42	
AT		-	CG1 I		1538			-3.05		.811	1.0		25.28	
ATO		•	D1 I		1538	3.22		-1.13	1 4	.269	1.0		22.28	
ATO		6 (	_		1538	4.37		-0.37	2 4	. 901	1.0		23.88	
ATO	- 0	7 C		`		0.76		~3.92		.292	1.0		7.19	
ATC	OM 60				1538	1.24		-5.03		. 035			5.59	
ATC	DM 61		_		L539	-0.19	3	-3.76	_	208	1.0		6.11	
ATO	M 61:		-	_	L <b>53</b> 9	-0.661	L	-4.94	_		1.00		6.13	
ATO				_	539	0.193		-5.28		934	1.00		5.25	
ATO			~~		539	1.214		-4.637		149	1.00		6.77	
ATO				S 1	540	-0.204				414	1.00	2	5.42	
ATO				S 1	540	0.467		6.327		862	1.00		5.62	
			3 LY	s ı	540	-0.552		6.716		092	1.00		3.38	
ATO			LY		540			7.283			1.00		1.15	
ATON		CD	LY		540	-1.573		6.303	11.		1.00		.13	
ATOM		CE			540	-2.528		6.943	12.		1.00		.23	
ATOM		NZ				-3.559	-	5.927	13.0		1.00		.69	
ATOM		C	LYS		340	-2.956	-	4.800	13.8				.08	
ATOM		o			40	1.609		7.705	10.0		1.00		.05	
ATOM	626	N	LYS		40	1.627	- :	8.600			.00		.37	
ATOM			HIS	-	41	2.545		7.538	9.1		00		.12	
ATOM		CA	HIS			3.666		3.440	10.9		.00	24	41	
ATOM	630	CB	HIS	15	41	4.772		3.228	11.0		.00	25.		
ATOM		CG	HIS	15	41	5.798	- 0	320	10.0		.00	21.		
ATOM	631	CD2	0	15	41	5.823		.320	10.0		.00	22.		
ATOM	632	ND1	HIS	154		6.939		. 522	9.4		. 00	21.	40	
	634	CE1	HIS	154		7 610	- 9	.268	10.8	43 1	.00	22.		
ATOM	635	NE2		154		7.619	-10	.389	10.69		.00	24.		
ATOM	637	C	HIS	154		6.966		.167	9.85	_	00			
ATOM	638	0	HIS			4.234	- 8	.328	12.49		00	27.		
ATOM	639	N		154		4.364		.239	13.05			25.		
ATOM	641	CA	LYS	154		4.560		476	13.06		00	26.		
ATOM	642		LYS	154	2	5.127	- 9 .	552			00	26.3		
ATOM	643	CB	LYS	154	2 !	5.515	-11.	002	14.40		00	30.0	7	
ATOM		CG	LYS	154		5.061	-17	252	14.69		00	31.3		
	644	CD	LYS	1542	-		-11.	252	16.07			42.7		
ATOM	645	CE	LYS	1542			-12.	_	16.29	4 1.		50.8		
ATOM	646	NZ	LYS	1542	•	.041	-13.	374	15.11	1 1.0		56.7		
MOTA	650	C	LYS		•	.511	-14.	763	15.424					
ATOM	651	0	LYS	1542		.342	-8.	652	14.624			61.2		
				1542	6	.519	-8.		15.711			27.6		
SSSD/55	145. vn1									. 1.0	טי :	26.8	3	



ATOM	652	N	ASN	1543	7.146	-8.445	13.585	1.00	27.20
ATOM	654	CA	ASN	1543	8.354	-7.642	13.735	1.00	25.50
MOTA	655	CB	ASN	1543	9.578	-8.431	13.260	1.00	25.59
ATOM	656	CG	ASN	1543	9.712	-9.767	13.974	1.00	22.64
ATOM	657	OD1	ASN	1543	9.522	-10.821	13.371	1.00	26.76
ATOM	658	ND2	ASN	1543	9.970	-9.727	15.273	1.00	25.56
ATOM	661	С	ASN	1543	8.374	-6.213	13.226	1.00	25.48
ATOM	662	0	ASN	1543	9.417	-5.692	12.842	1.00	24.58
ATOM	663	N	ILE	1544	7.209	-5.575	13.244	1.00	24.60
ATOM	665	CA	ILE	1544	7.065	-4.177	12.868	1.00	22.32
MOTA	666	CB	ILE	1544	6.524	-3.972	11.409	1.00	. 25.82
MOTA	667	CG2	ILE	1544	7.401	-4.720	10.403	1.00	24.24
ATOM	668	CG1	ILE	1544	5.057	-4.411	11.279	1.00	26.04
MOTA	669	CD1	ILE	1544	4.446	-4.121	9.901	1.00	23.20
MOTA	670	С	ILE	1544	6.075	-3.598	13.881	1.00	22.37
ATOM	671	0	ILE	1544	5.364	-4.345	14.559	1.00	21.68
ATOM	672	N	ILE	1545	6.111	-2.290	14.076	1.00	23.72
ATOM	674	CA	ILE	1545	5.169	-1.650	14.989	1.00	25.92
ATOM	675	CB	ILE	1545	5.602	-0.199	15.364	1.00	27.24
ATOM	676	CG2	ILE	1545	4.452	0.554	16.035	1.00	22.76
ATOM	677	CG1	ILE	1545	6.839	-0.219	16.285	1.00	25.57
ATOM	678	CD1	ILE	1545	6.591	-0.797	17.686	1.00	24.66
ATOM	679	C	ILE	1545	3.877	-1.612	14.179	1.00	26.03
MOTA	680	0	ILE	1545	3.823	-0.988	13.122	1.00	25.70
MOTA	681	N	ASN	1546	2.849	-2.293	14.669	1.00	24.79
MOTA	683	CA	ASN	1546	1.577	-2.354	13.956	1.00	25.51
MOTA	684	CB	ASN	1546	0.922	-3.727	14.137	1.00	25.17
ATOM	685	CG	ASN	1546	1.730	-4.839	13.539	1.00	21.67
MOTA	686	OD1	ASN	1546	1.856	-4.947	12.329	1.00	24.29
MOTA	687	ND2	ASN	1546	2.278	-5.686	14.384	1.00	22.24
MOTA	690	C	ASN	1546	0.578	-1.276	14.349	1.00	26.85
MOTA	691	0	ASN	1546	0.630	-0.724	15.453	1.00	28.67
MOTA	692	N	LEU	1547	-0.301	-0.956	13.407	1.00	27.70
ATOM	694	CA	LEU	1547	-1.357	0.019	13.622	1.00	27.64
ATOM	695	CB	LEU	1547	-1.945	0.481	12.284	1.00	24.87
ATOM	696	CG	LEU	1547	-3.173	1.400	12.337	1.00	23.25
ATOM	697	CD1	LEU	1547	-2.790	2.763	12.929	1.00	23.76
MOTA	698	CD2	LEU	1547	-3.757	1.569	10.923	1.00	23.47
ATOM	699	С	LEU	1547	-2.415	-0.771	14.396	1.00	27.27
ATOM	700	0	LEU	1547	-2.663	-1.952	14.103	1.00	25.27
ATOM	701	N	LEU	1548	-3.000	-0.130	15.400	1.00	27.94
ATOM	703	CA	LEU	1548	<b>-4.017</b>	-0.770	16.223	1.00	26.98
ATOM	704	CB	LEU	1548	-3.623	-0.735	17.708	1.00	24.65
MOTA	705	CG	LEU	1548	-2.327	-1.450	18.108	1.00	25.38
ATOM	706	CD1	LEU	1548	-2.189	-1.428	19.613	1.00	25.73
ATOM	707	CD2	LEU	1548	-2.337	-2.886	17.621	1.00	23.92
ATOM	708	C	LEU	1548	-5.369	-0.113	16.042	1.00	26.65
ATOM	709	0	LEU	1548	-6.392	-0.752	16.238	1.00	27.11
MOTA	710	N	GLY	1549	-5.378	1.163	15.684	1.00	25.04
MOTA	712	CA	GLY	1549	-6.643	1.855	15.516	1.00	25.47
ATOM	713	С	GLY	1549	-6.417	3.336	15.367	1.00	26.23
ATOM	714	0	GLY	1549	-5.267	3.781	15.287	1.00	28.41
MOTA	715	N	ALA	1550	-7.501	4.104	15.349	1.00	25.49
MOTA	717	CA	ALA	1550	-7.408	5.550	15.198	1.00	24.81

	ATOM	710											
	ATOM	718	CB	ALA	1550	-7.	176		_				
	ATOM	719	С	ALA	1550	-8.6	45	5.91			1.00	21.7	79
	ATOM	720	0	ALA	1550		770	6.27			1.00	25.5	
		721	N	CYS	1551	-8.4		5.702		726	1.00	24.0	
	MOTA	723	CA	CYS	1551			7.527			1.00	24.9	
	MOTA	724	CB	CYS	1551	-9.4		8.438	16.5		1.00		
	MOTA	725	SG	CYS		-9.2		8.932	17.9		1.00	26.8	
A	TOM	726	C	CYS	1551	-9.3		7.655	19.2			26.3	
		727	0	CYS	1551	-9.3	41	9.585			00	32.3	
A	TOM ;	728	••		1551	-8.36	51 1	0.338	15.5		.00	28.31	
		30			1552	-10.26		9.660	14.5		.00	28.42	2
			~-		1552	-10.19		0.671	14.5		.00	28.38	
					1552	-10.15		9.977	13.49		.00	31.26	
				THR :	1552	-11.40			12.09		.00	30.07	
		_		THR :	1552	-9.04		9.309	11.83		.00	29.64	
			C 7		L552	-11.35		3.945	12.05	3 1.	.00	28.65	
			o 1		552	-11 22		1.662	13.50		00		
		37 <u>1</u>	_		.553	-11.29		2.722	12.87	_		33.31	
AT		19 (			553	-12.42		.309	14.21			31.94	
ΑT		_				-13.59	3 12	.158	14.24			36.09	
AT	OM 74	_			553	-14.864	11	.299	14.14			39.26	
ATO	OM 74	_			553	-14.932	10	.436	12.88			36.61	
ATO	OM 74	-	_		553	-14.762	11	.247	11.601			37.72	
ATO	OM 74	. •			553	-15.491		.210	11.001		-	38.41	
ATC	_				553	-13.798		.858	11.363			7.88	
ATC		_	GI			-13.671		.079	10.770			7.67	
ATO			GI	N 15		-13.150	10	750	15.451			1.28	
ATO	-	••	,	P 15		-14.282	12.	758	16.513	1.0		1.37	
ATO			A AS	P 15		-14.487	14.	246	15.243	1.0	_	4.93	
ATO			3 AS	P 15		15.828			16.281	1.0		8.05	
	_		AS.			17.007		009	16.975	1.0		0.80	
ATO			1 AS			17.007	15.	281	16.067	1.0		5.88	
ATO		OD	2 AS			17.921	16.	019	16.491	1.0			
ATON		С	ASI			17.016	14.	776 ]	14.925	1.00		3.89	
ATOM		0	ASI			13.367	15.	366 1	17.316	1.00	- •	3.98	
ATOM		N	GLY			13.556	15.0		8.502			.04	
ATOM	760	CA	GLY	-		12.205	15.8		6.860	1.00	_	.73	
ATOM	761	C				11.080	15.9		7.756	1.00		.30	
ATOM		ō	GLY			-9.761	15.7		7.052	1.00		.32	
ATOM	763	N	GLY			9.740	15.4		7.03Z	1.00	_	.69	
ATOM			PRO	155		8.644	15.7		5.848	1.00		.71	
ATOM	765	CD	PRO	155	6 -	8.585	15.9		7.782	1.00	39	.49	•
ATOM	_	CA	PRO	155		7.298	15.5		9.235	1.00		36	
ATOM	766 767	CB	PRO	1556	5 -	6.405			7.250	1.00	38.		
ATOM	767	CG	PRO	1556	5 -	7.226	15.7		3.470	1.00	38.		
	768	C	PRO	1556	5 -	7.140	16.5		388	1.00	41.		
ATOM	769	0	PRO	1556		7.140	14.15		. 746	1.00	36.		
ATOM	770	N	LEU	1557		7.606	13.20		.371	1.00	37.		
ATOM	772	CA	LEU	1557		6.447	14.01	.7 15		1:00	37.	74	
ATOM	773	CB	LEU			5.201	12.71			1.00	36.		
ATOM	774	CG	LEU	1557	_	5.528	12.88				34.		
ATOM	775	CD1		1557		004	11.62			1.00	32.4		
ATOM	776	CD2	LEU	1557	-6	.146	10.65	_		1.00	30.8		
ATOM	777		LEU	1557	-4	.283	12.01			1.00	26.2	8	
ATOM	778	C	LEU	1557	- 5	.290	11.92			1.00	25.5	5	
ATOM		0	LEU	1557	- 4	.229			961 1	.00	33.6		
ATOM	779	N	TYR	1558	_		12.410		369 1	00	33.6		
014	781	CA	TYR	1558	-4	.902	10.724		319 1	.00	31.9		
CCCD/r-	• • •				•	. 202	9.863	17.		.00	31.8		
SSSD/55	145. v01											_	





							9.500	18.462	1.00		
MOTA	782	CB	TYR	1558		5.614 5.710	10.638	19.461	1.00		
ATOM	783	CG	TYR	155		6.644	10.608	20.499	1.00		
MOTA	784	CD1	TYR	155			11.670	21.394	1.00	38.	
ATOM	785	CE1	TYR	155		6.757	11.759	19.349	1.00	38	
ATOM	786	CD2	TYR	155		4.883	12.824	20.235	1.00		. 33
ATOM	787	CE2	TYR	155	_	4.985	12.781	21.254	1.00		.70
ATOM	788	CZ	TYR	155	-	5.924 6.040	13.867	22.104	1.00	3 42	.66
ATOM	789	OH	TYR	155		-4.607	8.604	16.345	1.0		.08
MOTA	791	C	TYR	155	-		7.937	15.857	1.0		.28
MOTA	792	0	TYR	155		-5.527 -3.328	8.336	16.116	1.0		.34
MOTA	793	N	VAL	155		-2.934	7.132	15.403	1.0		.39
ATOM	795	CA	VAL	15	-	-1.830	7.401	14.364	1.0		.17
ATOM	796	CB	VAL	15		-1.830	6.103	13.648		0 26	. 25
MOTA	797	CG1	VAL	15		-1.463 -2.297	8.461	13.360	1.0		.56
ATOM	798	CG2	JAV	15			6.226	16.498	1.0		5.14
ATOM	799	С	VAL	15		-2.411	6.522	17.120	1.0		3.04
ATOM	800	0	VAL	_		-1.396 -3.164	5.171	16.78	3 1.0		5.28
ATOM		N	ILE	_	60	-2.832	4.208	17.83			4.81
ATOM		CA	ILE	_	60	-4.133	3.669		6 1.		4.63
ATOM		CB	ILE		60	-3.790	2.812		8 1.		0.93
ATOM		CG2		_	60	-5.044	4.854				2.94
ATOM		CG1			60	-6.499	4.502	19.02			5.34
MOTA		CD1			560	-1.994	3.051	17.28			6.38
ATOM		С	IL		560	-2.429	2.30	16.39			6.14
MOTA		0	IL		560	-0.782	2.91	17.80			27.31
ATO		N	AV		561	0.112	1.85	2 17.35			27.32
OTA	M 812	CA	VA		561	1.309	2.43	5 16. <b>5</b> 7			25.01 19.39
ATO	M 813	CB	VA		561	0.785	3.22	0 15.3			26.08
OTA	M 814				561 561	2.170	3.34	0 17.3			25.89
ATO					561	0.615	1.02	9 18.5			25.64
ATO	M 816		VF		.561	0.364		3 19.7			24.49
ATO	M 817		V		562	1.288		6 18.2		.00	25.00
ATC			GI		1562	1.806	-0.94			00	23.69
ATC					1562	2.357	-2.23			00	24.29
ATO					1562	1.272	-3.1			1.00	27.65
ATO					1562	1.814	-4.3	93 17.5		1.00	29.50
TA					1562	1.218	-5.4			1.00	32.34
TA				LU	1562	2.832				1.00	27.27
TA		_	_	LU	1562	2.84				1.00	26.18
TA		_		LU	1562	3.59				1.00	30.39
	OM 82			YR	1563	2.82				1.00	32.48
	OM 82			YR	1563	3.71			750	1.00	33.91
	OM 83	_		YR	1563	2.93			928	1.00	34.93
	OM 83			ryr	1563	3.78			871	1.00	34.50
				ryr	1563	4.60			967	1.00	37.77
				TYR	1563	5.37	_		108	1.00	33.54
				TYR	1563	3.75			.205	1.00	34.94
				TYR	1563	4.5	_		. 128	1.00	37.22
		-		TYR	1563	5.3			.206	1.00	45.36
	-	_	OH	TYR	1563	6.0			.730	1.00	31.53
		-	C	TYR	1563	4.8			. 895	1.00	30.43
			0	TYR	1563	3 4.7	_		.761	1.00	32.28
			N	ALA	1564	6.0	82 -0.	444 22			
₽	MOTA	, 4 4									

••	O 36/0 /	835					
					13	30	
ATOM ATOM ATOM	844 845 846 847	CA CB C	ALA ALA ALA ALA	1564 1564 1564 1564	7.326 8.308 7.897	-1.167 -0.957 -0.608	23.020 21.86: 24.334
ATOM	848	N	SED	1565	8.563	0.427	24 345

AT 26 1.00 32.59 AT 63 1.00 30.11 AT 34 1.00 31.81 ATOM N 0.427 SER 24.345 1565 1.00 7.619 34.11 ATOM 850 -1.296 CA 25,434 SER 1565 1.00 ATOM. 8.039 34.09 851 -0.853 CB 26.763 SER 1565 1.00 35.05 7.400 ATOM 852 -1.725 OG 27.829 SER 1565 1.00 30.13 7.689 ATOM 854 -3.084 C 27.579 SER 1565 1.00 38.17 ATOM 9.526 855 -0.769 SER 27.041 0 1565 1.00 35.03 MOTA 9.947 856 -0.001 N 27.902 LYS 1566 1.00 ATOM 10.321 37.12 -1.557 858 CA 26.330 1566 LYS 1.00 11.756 34.55 ATOM 859 -1.559 CB LYS 26.562 1566 1.00 12.291 33.48 ATOM 860 -2.990 CG LYS 26.508 1566 1.00 11.674 31.90 MOTA 861 -3.865 CD 27.586 LYS 1566 1.00 12.162 28.63 MOTA 862 -5.287 CE LYS 27.508 1566 1.00 34.97 ATOM 11.763 863 -6.042 NZ 28.761 LYS 1566 1.00 12.288 36.82 MOTA 867 -7.433 C LYS 28.748 1566 1.00 12.567 41.32 MOTA 868 -0.613 0 LYS 25.691 1566 1.00 34.98 13.785 ATOM 869 -0.740 N GLY 25.607 1567 1.00 38.03 ATOM 11.892 871 0.338 CA 25.049 GLY 1567 1.00 12.582 36.00 ATOM 872 1.322 C GLY 24.222 1567 1.00 ATOM 13.245 34.14 873 0.864 0 22.933 GLY 1567 1.00 ATOM 12.975 32.01 874 -0.222 N 22.439 ASN 1568 1.00 14.091 31.95 ATOM 876 CA 1.719 ASN 22.360 1568 1.00 14.774 33.51 ATOM 877 1.375 CB ASN 21.121 1568 1.00 34.20 MOTA 15.203 878 2.627 CG 20.332 ASN 1568 1.00 34.07 ATOM 16.420 879 3.321 OD1 20.910 ASN 1568 1.00 17.453 35.09 ATOM 880 2.709 ND2 21.156 ASN 1568 1.00 ATOM 34.36 16.317 883 4.624 21.066 C ASN 1568 1.00 ATOM 38.38 15.927 884 0.401 0 ASN 21.325 1568 1.00 16.490 33.38 ATOM 885 0.315 N LEU 22.414 1569 1.00 34.93 16.276 ATOM 887 -0.317 CA LEU 20.263 1569 1.00 31.11 ATOM 17.333 888 -1.316 CB 20.298 LEU 1569 1.00 17.437 30.44 MOTA 889 -2.008 CG 18.928 LEU 1.00 1569 ATOM 18.438 29.46 -3.148 890 18.741 CD1 LEU 1569 1.00 18.285 ATOM 29.01 891 -4.219 CD2 19.840 LEU 1569 1.00 18.263 28.81 ATOM 892 -3.740 C 17.338 LEU 1569 1.00 18.706 26.62 ATOM 893 -0.805 0 20.762 LEU 1569 1.00 19.400 30.16 ATOM 894 -1.501 N 21.496 ARG 1570 1.00 27.32 19.097 ATOM 896 0.396 CA 20.344 ARG 1570 1.00 30.74 20.386 ATOM 897 0.951 CB 20.758 ARG 1570 1.00 20.597 33.72 ATOM 2.349 898 CG ARG 20.160 1.00 1570 32.82 21.873 ATOM 899 3.009 CD ARG 20.662 1.00 1570 36.90 ATOM 21.966 900 4.481 NE 20.332 ARG 1570 1.00 39.32 20.749 ATOM 5.222 902 CZ 20.664 ARG 1570 1.00 50.32 20.376 ATOM 903 5.600 NH1 21.889 ARG 1.00 1570 21.118 51.90 MOTA 906 5.316 NH2 22.960 ARG 1.00 1570 50.15 ATOM 19.246 909 6.284 C ARG 22.033 1.00 1570 53.67 ATOM 20.434 910 1.022 0 ARG 22.298 1.00 1570 35.75 ATOM 21.324 911 0.444 N GLU 22.939 1571 1.00 35.67 19.444 MOTA 913 1.695 CA 22.880 GLU 1.00 1571 19.331 35.56 ATOM 914 1.835 CB 24.328 GLU 1.00 1571 36.50 18.055 ATOM 915 2.607 CG 24.667 GLU 1571 1.00 18.061 39.08 4.056 24.208 1.00 46.75

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ATOM	916	CD	GLU	1571	16.694	4.721	24.311	1.00	51.36
MOTA	917	OEl	GLU	1571	15.676	3.996	24.417	1.00	55.22
MOTA	918	OE2	GLU	1571	16.635	5.972	24.267	1.00	53.59
MOTA	919	C	GLU	1571	19.314	0.469	25.022	1.00	34.82
ATOM	920	0	GLU	1571	20.018	0.242	26.013	1.00	35.05
ATOM	921	N	TYR	1572	18.520	-0.441	24.469	1.00	33.35
ATOM	923	CA	TYR	1572	18.366	-1.796	24.986	1.00	31.83
ATOM	924	CB	TYR	1572	17.365	-2.544	24.102	1.00	30.77
ATOM	925	CG	TYR	1572	17.170	-4.008	24.408	1.00	28.50
ATOM	926	CD1	TYR	1572	16.193	-4.420	25.313	1.00	30.48
ATOM	927	CE1	TYR	1572	15.977	-5.760	25.574	1.00	30.97
ATOM	928	CD2	TYR	1572	17.933	-4.985	23.772	1.00	26.14
ATOM	929	CE2	TYR	1572	17.725	-6.329	24.027	1.00	26.21
ATOM	930	CZ	TYR	1572	16.742	-6.708	24.935	1.00	30.30
ATOM	931	ОН	TYR	1572	16.518	-8.041	25.214	1.00	33.52
ATOM	933	C	TYR	1572	19.692	-2.556	25.044	1.00	34.83
ATOM	934	0	TYR	1572	19.959	-3.308	25.992	1.00	34.93
ATOM	935	N	LEU	1573	20.517	-2.370	24.020	1.00	34.34
ATOM	937	CA	LEU	1573	21.803	-3.053	23.961	1.00	35.38
ATOM	938	CB	LEU	1573	22.357	-3.027	22.531	1.00	32.71
ATOM	939	CG	LEU	1573	21.669	-3.891	21.464	1.00	29.16
ATOM	940	CD1	LEU	1573	22.161	-3.503	20.087	1.00	26.98
ATOM	941	CD2	LEU	1573	21.932	-5.351	21.710	1.00	28.85
ATOM	942	С	LEU	1573	22.799	-2.420	24.933	1.00	37.54
ATOM	943	0	LEU	1573	23.511	-3.123	25.659	1.00	36.67
ATOM	944	N	GLN	1574	22.814	-1.092	24.969	1.00	37.90
MOTA	946	CA	GLN	1574	23.729	-0.368	25.838	1.00	39.77
MOTA	947	СВ	GLN	1574	23.624	1.138	25.572	1.00	40.09
ATOM	948	CG	GLN	1574	24.208	1.549	24.217	1.00	42.28
ATOM	949	CD	GLN	1574	24.030	3.018	23.896	1.00	44.28
ATOM	950	OE1	GLN	1574	23.362	3.755	24.615	1.00	47.55
ATOM	951	NE2	GLN	1574	24.613	3.448	22.790	1.00	46.09
ATOM	954	С	GLN	1574	23.490	-0.697	27.310	1.00	40.75
MOTA	955	0	GLN	1574	24.440	-0.939	28.059	1.00	41.29
MOTA	956	N	ALA	1575	22.220	-0.783	27.696	1.00	40.10
ATOM	958	CA	ALA	1575	21.842	-1.088	29.069	1.00	38.81
ATOM	959	CB	ALA	1575	20.349	-0.819	29.273	1.00	35.69
ATOM	960	С	ALA	1575	22.192	-2.514	29.503	1.00	40.63
ATOM	961	0	ALA	1575	22.098	-2.843	30.690	1.00	43.39
ATOM	962	N	ARG	1576	22.602	-3.357	28.561	1.00	38.39
MOTA	964	CA	ARG	1576	22.945	-4.729	28.896	1.00	37.69
MOTA	965	CB	ARG	1576	22.034	-5.689	28.137	1.00	38.16
MOTA	966	CG	ARG	1576	20.594	-5.547	28.589	1.00	37.89
ATOM	967	CD	ARG	1576	19.622	-6.281	27.711	1.00	37.36
ATOM	968	NE	ARG	1576	18.267	-6.255	28.265	1.00	34.99
ATOM	970	CZ	ARG	1576	17.565	-5.150	28.484	1.00	36.94
ATOM	971	NH1	ARG	1576	18.083	-3.960	28.209	1.00	36.18
ATOM	974	NH2	ARG	1576	16.310	-5.237	28.909	1.00	40.93
ATOM	977	C	ARG	1576	24.413	-5.073	28.704	1.00	38.93
ATOM	978	o	ARG	1576	24.801	-6.249	28.699	1.00	39.75
ATOM	979	N	ARG	1577	25.233	-4.036	28.570	1.00	39.21
MOTA	981	CA	ARG	1577	26.671	-4.196	28.413	1.00	38.97
ATOM	982	СВ	ARG	1577	27.307	-2.870	28.000	1.00	36.06
ATOM	983	CG	ARG	1577	26.992	-2.408	26.610	1.00	36.41
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	OM 98	4 0	D A	RG 157	7 27.6	95 1 0.			
AT		5 N	E Al	RG 1577					36.17
AT		7 C	Z AI	RG 1577					
AT		8 N	H1 AF						39.00
ATO		1 N	H2 AF						38.88
ATO		4 C	AF						37.76
ATO		5 0							40.59
ATC	DM 996	5 N							38.52
ATC	M 997	7 CI			29.07				43.19
ATC		C.			28.95				44.84
ATO	M 999	CE			30.06			1.00	45.06
ATO	M 100	o ca				_			44.86
ATO	M 100	ı c	PRO	_	30.43			1.00	44.56
ATO	M 100	2 0	PRO		29.51				44.93
ATO		3 N	PRO		29.80				43.13
ATO		4 CD			29.649			1.00	47.61
ATO	M 100				29.319			1.00	48.39
ATON	4 100				30.173			1.00	48.74
ATON	1 100		PRO		30.138			1.00	49.73
MOTA	1 1008	3 C	PRO	_	29.027			1.00	49.21
ATOM			PRO		31.591			1.00	49.67
ATOM		N	GLU		32.483			1.00	52.07
ATOM		CA	GLU		19.165			1.00	64.83
ATOM	1013		GLU		20.603		32.491	1.00	64.82
ATOM	1014		GLU		20.969		33.784	1.00	67.61
ATOM	1015		GLU	1592	21.448		32.335	1.00	63.99
MOTA	1016		GLU	1593	22.653	-6.336	32.098	1.00	65.67
MOTA	1018		GLU	1593	20.821	~7.575	32.485	1.00	62.41
ATOM	1019		GLU	1593	21.534	-8.844	32.342	1.00	61.23
MOTA	1020	С	GLU	1593	20.595	-10.017	32.600	1.00	61.20
MOTA	1021	0	GLU	1593	22.141	-8.953	30.944	1.00	59.26
ATOM	1022	N	GLN	1594	21.494	-8.631	29.945	1.00	59.84
ATOM	1024	CA	GLN	1594	23.388	-9.405	30.888	1.00	57.94
ATOM	1025	СВ	GLN	1594	24.101	-9.558	29.625	1.00	54.91
ATOM	1026	CG	GLN	1594	25.501	-10.141	29.865		55.13
ATOM	1027	CD	GLN	1594	26.439	-9.252	30.679		56.93
ATOM	1028	OE1	GLN	1594	27.682	-9.997	31.180		59.60
ATOM	1029	NE2	GLN	1594	28.241	-10.858	30.488		58.45
MOTA	1032	С	GLN	1594	28.117	-9.662	32.393		58.95
MOTA	1033	0	GLN	1594	23.331	-10.438	28.640		52.30
ATOM	1034	N	LEU	1595	22.637	-11.389	29.025		52.03
ATOM	1036	CA	LEU	1595	23.438	-10.091	27.366		9.60
ATOM	1037	СВ	LEU	1595	22.782	-10.836	26.308		15.16
ATOM	1038	CG	LEU	1595	22.459	-9.907	25.135	_	1.36
ATOM	1039	CD1	LEU	1595	21.463	-8.815			9.43
MOTA	1040	CD2	LEU	1595	21.617	-7.583			6.21
ATOM	1041	C	LEU		20.060	-9.389			4.91
MOTA	1042	0	LEU	1595	23.747	-11.900			3.30
MOTA	1043	N		1595	24.953	-11.675			3.62
ATOM	1045	CA	SER	1596	23.230	-13.081			2.92
ATOM	1046	CB	SER	1596	24.085	-14.150			1.86
ATOM	1047	OG			23.410	-15.502			0.86
ATOM	1047	C			22.188				7.88
ATOM	1050	0		1596	24.322	-13.914			7.88 1.59
		•	SER	1596	23.657				1.59
SSSD/55	145 vn1						-	4.	

ATOM	1051	N	SER	1597	25.275	-14.637	23.018	1.00	39.60	
ATOM	1053	CA	SER	1597	25.557	-14.518	21.603	1.00	39.74	
ATOM	1054	CB	SER	1597	26.729	-15.409	21.223	1.00	41.38	
ATOM	1055	OG	SER	1597	27.824	-15.147	22.077	1.00	50.59	
ATOM	1057	С	SER	1597	24.315	-14.921	20.818	1.00	38.16	
MOTA	1058	0	SER	1597	24.036	-14.353	19.769	1.00	38.03	
MOTA	1059	N	LYS	1598	23.560	-15.891	21.327	1.00	36.40	
MOTA	1061	CA	LYS	1598	22.362	-16.312	20.634	1.00	35.97	
MOTA	1062	СВ	LYS	1598	21.791	-17.594	21.228	1.00	36.69	
MOTA	1063	CG	LYS	1598	20.989	-18.402	20.198	1.00	40.42	
MOTA	1064	CD	LYS	1598	20.164	-19.499	20.838	1.00	40.37	
MOTA	1065	CE	LYS	1598	19.792	-20.572	19.829	1.00	46.34	
MOTA	1066	NZ	LYS	1598	20.993	-21.338	19.362	1.00	45.29	
MOTA	1070	С	LYS	1598	21.324	-15.194	20.696	1.00	37.49	
MOTA	1071	0	LYS	1598	20.567	-14.983	19.738	1.00	38.10	
ATOM	1072	N	ASP	1599	21.316	-14.458	21.807	1.00	35.21	
MOTA	1074	CA	ASP	1599	20.380	-13.352	21.983	1.00	34.02	
MOTA	1075	CB	ASP	1599	20.556	-12.686	23.346	1.00	37.78	
MOTA	1076	CG	ASP	1599	19.970	-13.493	24.483	1.00	40.05	
MOTA	1077	OD1	ASP	1599	20.270	-13.143	25.642	1.00	42.73	
ATOM	1078	OD2	ASP	1599	19.204	-14.450	24.235	1.00	42.39	
ATOM	1079	C	ASP	1599	20.633	-12.306	20.922	1.00	32.84	
MOTA	1080	0	ASP	1599	19.694	-11.779	20.311	1.00	30.59	
MOTA	1081	N	LEU	1600	21.912	-11.999	20.724	1.00	31.11	
ATOM	1083	CA	LEU	1600	22.323	-10.998	19.744	1.00	32.17	
MOTA	1084	CB	LEU	1600	23.823	-10.722	19.875	1.00	32.30	
MOTA	1085	CG	LEU	1600	24.275	-10.162	21.235	1.00	31.08	
MOTA	1086	CD1	LEU	1600	25.794	-9.931	21.242	1.00	30.59	
ATOM	1087	CD2	LEU	1600	23.549	-8.863	21.514	1.00	28.89	
ATOM	1088	С	LEU	1600	21.949	-11.390	18.311	1.00	30.77	
MOTA	1089	0	LEU	1600	21.352	-10.601	17.574	1.00	29.87	
MOTA	1090	N	VAL	1601	22.269	-12.623	17.933	1.00	30.19	
MOTA	1092	CA	LAV	1601	21.954	-13.115	16.602	1.00	29.25	
MOTA	1093	CB	VAL	1601	22.593	-14.497	16.349	1.00	31.27	
MOTA	1094	CG1	VAL	1601	22.355	-14.936	14.914	1.00	31.60	
MOTA	1095	CG2	VAL	1601	24.093	-14.434	16.622	1.00	31.91	
ATOM	1096	С	VAL	1601	20.438	-13.181	16.405	1.00	29.06	
ATOM	1097	0	VAL	1601	19.946	-12.914	15.310	1.00	27.71	
ATOM	1098	N	SER	1602	19.702	-13.511	17.468	1.00	29.10	
ATOM	1100	CA	SER	1602	18.243	-13.585	17.400	1.00	29.29	
ATOM	1101	CB	SER	1602	17.680	-14.189	18.679	1.00	30.81	
ATOM	1102	OG	SER	1602	16.266	-14.074	18.692	1.00	35.78	
ATOM	1104	C	SER	1602	17.649	-12.199	17.156	1.00	28.98	
ATOM	1105	0	SER	1602	16.662	-12.039	16.426	1.00	26.82	
MOTA	1106	N	CYS	1603	18.274	-11.202	17.765	1.00	29.06	
ATOM	1108	CA	CYS	1603	17.870	-9.823	17.599	1.00	29.22	
ATOM	1109	CB	CYS	1603	18.784	-8.943	18.438	1.00	29.66	
ATOM	1110	SG	CYS	1603	18.575	-7.212	18.103	0.50	23.69	PRT1
ATOM	1111	C	CYS	1603	17.988	-9.422	16.112	1.00	29.23	
ATOM	1112	0	CYS	1603	17.087	-8.796	15.552	1.00	27.52	
MOTA	1113	N	ALA	1604	19.113	-9.778	15.491	1.00	27.87	
MOTA	1115	CA	ALA	1604	19.376	-9.484	14.077	1.00	26.37	
MOTA	1116	CB	ALA	1604	20.783	-9.941	13.690	1.00	23.88	
MOTA	1117	С	ALA	1604	18.349	-10.203	13.223	1.00	25.82	

							-	134				
	ATOM	1118	0	ALA	1604							
	ATOM	1119	N		1605			-9.	631 1	2.289	1.00	25.04
	ATOM	1121	CA		1605			-11.	468 13	3.544	1.00	-0.04
	ATOM	1122	CB		1605	17.		-12.	276 12	2.827	1.00	
	ATOM	1123	CG		.605	17.0		-13.	662 13	.456	1.00	27.81
	ATOM	1124	CD1		605	15.9		-14.	515 12	.886	1.00	26.66
	ATOM :	1125	CE1		605	16.1	.11	-15.	141 11	.640	1.00	30.75
	MOT	1126	CD2		605	15.0		-15.9	944 11	.126	1.00	30.20
	TOM 1	1127	CE2		605	14.7		-14.7	07 13	. 596	1.00	30.03
	TOM 1	128	CZ		605	13.7		-15.5	00 13	. 097	1.00	30.73
	TOM 1	129	O11		505	13.9		-16.1	17 11	867	1.00	30.71
		131	~		505	12.9		-16.9	28 11.	417	1.00	30.93
	TOM 1	132	^	n		15.74	18	-11.6		775	1.00	32.31
		133			05	15.14	17	-11.5		702	1.00	26.15
		135 (			06	15.24		-11.2				26.64
	COM 1				06	13.92		-10.58		_	1.00	25.48
	OM 1				06	13.58		-10.26	9 15.		1.00	26.86
	'OM 11					13.35	7	-11.50	8 16.		1.00	26.83
	OM 11					13.15	1	-11.16		<b>-</b>		25.84
AT						12.20	2 .	-10.47				30.86
AT	OM 11					14.05	5.	-11.63	1 18.6			31.87
AT		44 0				13.835	5 .	-9.31	0 13.1			31.67
ATO	OM 11		V.			12.831		-9.05	B 12.5			27.52
ATO	OM 114					14.904		-8.52	13.2			26.05
ATC	DM 114			_		14.963		-7.303	12.4			6.68
ATC	M 114	19 CG		•		16.225		-6.485				5.66
ATO						16.363		-5.274				8.50
ATO			VA			16.151		-6.031	14.2			6.04
ATO		2 0	VA:			14.934		-7.641	10.93			4.45
ATO		3 N	AL			14.184		-7.033				4.89
ATO		5 CA	AL			15.738		8.619	10.52	_		5.86
ATON		6 CB	ALA			15.773	-	9.039	9.12			5.24
ATOM		7 C	ALA			16.813	- 1	0.117	8.92			2.95
ATOM		3 0	ALA			14.383	-	9.541	8.67			. 24
ATOM		N	ARG			13.963	-	9.319	7.53			. 71
ATOM			ARG			13.676	- 1	0.216	9.58		00 27	.48
ATOM		CB	ARG			2.327		0.708	9.30			.10
ATOM		CG	ARG	1609		1.840		1.640	10.397	1.0		.55
ATOM		CD	ARG	1609		2.407	-13	3.005	10.290	1.0		.53
ATOM	1165	NE	ARG	1609		1.537	-13	3.931	11.056			. 05 . 28
ATOM	1167	CZ	ARG	1609		0.849	-14	1.874	10.190	1.0	-	. 28
ATOM	1168	NH1	ARG	1609		9.974	-15	.771	10.632	1.0		
ATOM	1171	NH2	ARG	1609		9.678	-15	.834	11.928	1.0		
ATOM	1174	С	ARG	1609		9.416	-16	.620	9.784	1.0		
ATOM	1175	0	ARG	1609	1.1	1.329	- 9	.569	9.124	1.0	_	
ATOM	1176	N	GLY	1610		.469	- 9	.621	8.231	1.0		
ATOM	1178	CA	GLY	1610	11	418		. 565	9.996	1.00	-	
MOTA	1179	C	GLY	1610		.555	- 7	<b>.4</b> 06	9.870	1.00	- •	
ATOM	1180	0	GLY			.800	-6.	. 747	8.512	1.00		
ATOM	1181	N	MET	1610	9	.855	-6.	424	7.772	1.00		
MOTA	1183	CA	MET	1611	12	.076	-6.	589	8.163			
ATOM	1184	CB	MET	1611		.456	-5.	989	6.888	1.00		
ATOM	1185	CG	MET	1611		. 956	-5.	710	6.849	1.00		
ATOM	1186	SD	MET	1611		. 398	-4.	542	7.729	1.00		.8
			. 151	1611	13.	478	-3.	006	7.426		22.6	
SSSD/55	145 v01									1.00	25.2	3



											25	,
							-2.6	88	5.675	1.00		) :
- 5016	1187	CE	MET	1611	13.	817	-6.8		5.681	1.00	0	) :
MOTA	1188	C	MET	1611	12. 11.	0.30 673	-6.3		4.633	1.00	_	4
MOTA	1189	0	MET	1611	11.	130	-8.3		5.822	1.00		4
MOTA	1190	N	GLU	1612	12.	720	-9.		4.733	1.00		6
MOTA	1192	CA	GLU	1612	11.	755	-10.	494	5.121	1.00		۵
MOTA	1193	CB	GLU	1612	12.	018	-11.	488	4.009	1.00		
MOTA	1194	CG	GLU	1612	11.	703	-12.	931	4.450			
MOTA	1195	CD	GLU	1612	11.	.812	-13.	212	5.636			1
MOTA	1196	OE1	GLU	1612	11	.557	-13.	791	3.611			70
MOTA	1197	OE2	GLU	1612	12	.154	-8.	829	4.415			70
MOTA	1198	C	GLU	1612	10	.267	- 8	.753	3.252	1.0		50 e E
MOTA	1199	0	GLU	1612		.860	-8	.723	5.46	5 1.0		
ATOM	1200		TYR	1613		.463	-8	.501	5.29	4 1.0		94
MOTA			TYR	1613		.037	-8	.586	6.65	0 1.0		00
MOTA			TYR	1613		.314		.281	6.54	9 1.0		93
MOTA			TYR	1613		5.841		.245	6.09	7 1.		14
MOTA				1613		4.945	- 8	.962	5.96	3 1.		. 14
ATOM				1613		3.582		7.018	6.86			.81
MOTA						5.347		5.718	6.73		-	.45 .28
MOTA		_				3.979		7.697	6.28	-		.95
IOTA			TYI	1613		3.112 1.775		7.411	6.1			.57
OTA			TY					7.138	4.6	-		.72
ATO		_	TY			7.803 7.022		7.024	3.6		-	2.16
ATO!		_	TY			8.460		6.101	5.1		• -	2.60
OTA			LE			8.460		4.755	4.6			2.56
OTA			LE	U 161		9.175		3.772	5.4			4.92
ATC			LE			8.57	-	3.415	6.8		_	1.46
OTA			LE			9.53		-2.541	7.5			1.40
ATC			)1 LI	EU 161		7.21		-2.71	6.0		_	3.76
)TA )TA			02 L	2ប 161		8.69		-4.683	ვ 3.∵		-	3.84
TA		21 C	L	EU 163		7.97	-	-4.07	72.		_	3.48
TA		22 0	L	EU 163		9.80		-5.31	42.			22.70
		223 N	A	LA 16		10.23	32	-5.34	0 1.	_		21.52
			A A	LA 16		11.59	91	-6.01	9 1.		_	22.87
			B A		15	9.1		-6.06	3 0.	_		24.23
	_	227	. F		15	8.8		-5.59	1 -0.	.581		22.76
			) [		15	8.6		-7.17	76 1	.015	-	22.88
			. •		516	7.6		-7.9	54 0	.295		21.39
			CA 1	J	516	7.3		-9.2	51 <sup>1</sup>	.039		26.24
		232			616	6.4		-9.0	36 .2	.102	1.00	24.88
			OG		616	6.3	360	-7.1	31 0	.044	1.00	24.73
		1235	C		616	5.6	635	-7.3	58 -0	.927	1.00	23.82
		1236	0		616		104	-6.1		.927	1.00	22.47
		1237	N		.617	Δ.	970	-5.2	87	0.810	1.00	23.62
		1239	CA		.617		455	-4.9	14	2.199	1.00	27.16
		1240	CB		1617		792	-6.0	72	2.927	1.00	30.84
	MOTA	1241	CG		1617		551	· -6.	487	2.169	1.00	33.57
	MOTA	1242	CD		1617	1	810	-7.	602	2.852	1.00	44.30
	MOTA	1243	CE		1617	2	484	-8.	894	2.653	1.00	23.56
•	ATOM	1244	NZ		1617	Z.	.346	-4.	034	0.035	1.00	25.16
	MOTA	1248	С		1617		.639	-3.	030	0.091	1.00	24.69
	MOTA	1249	0	LYS	1617		.495	-4.	066	0.638	1.00	24.04
	ATOM	1250	N	LYS	1618		.953		943	-1.468	1.00	6-2.01
	MOTA	1252	CA	LYS	1618	9	. , , ,					
	F1. 0											

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ATOM 1253 CB LVC 1620	
ATOM 1254 CC 1618 5.863 53.503	
ATOM 1255 CD 415 1618 5.775 3.492	
ATOM 1356 - 113 1618 5 567 - 3.709	20.56
ATOM -4.942 -3.345	23.14
ATOM	93.31
1261 C IVC 150 4.431 -5.821 5	1.00 32.98
1262 O LVS 1616 -1.686 O THE	1.00 36.73
1263 N CVC 7.557 -0.606	1.00 24.01
110H 1265 CA 7.689 -1 040	1.00 23.73
ATOM 1266 CD 1619 8.108 0.573	1.00 25.91
ATOM 10-1 1.418	
ATOM 100 SG CYS 1619 70.885 2.792	
ATOM 100 CYS 1619 0.313 4.064	
1269 O CVC 3.631 -0.630	1.00 28.14
1270 N Trn 10.304 -1.630	1.00 23.07
1272 CA TIN 10.170 0.573	1.00 20.98
ATOM 1273 CB 1620 11.604 1.363	1.00 22.95
ATOM 1274 CC2 1620 12.202 1 1.524	1.00 23.81
ATOM 10- 100 1620 13 cm	
ATOM 100 ILE 1620 10 10 1.995 0.506	-4.50
-270 CD1 1th 1200 () 720 -	
	1.00 23.13
1278 0 11.633 1 720	.00 25.37
1279 N HTC 10.981 2.763	.00 24.70
1281 CA HTC 12.348 1.297	.00 25.21
1282 CD 12.427	.00 25.62
ATOM 1283 CC 113 1621 13:181 5:057 1	.00 25.53
ATOM 1284 CD2 115 1621 13.004 1.237 6.132 1	
ATOM 1205 1521 12 256 7.528 1	
ATOM 1335 NDI HIS 1621 13 45 1.260 8.603 1	
ATOM 3.011 7 927	/-
- 100 NEX 1170 3 222	00 26.62
1290 C HTC 12.439 2 197	
1291 0 470 13.073 3.401	
1292 N NPG 12.528 4 405	<sup>00</sup> 26.36
1294 (7)	25.89
ATOM 1295 CD 4.341 1.0	00 25.35
ATOM 1296 CO ARG 1622 14 268 4 140 1.0	
ATOM 3.540 1.0	
ATOM 100 ARG 1622 13 00 5.444 2.175 1.00	
ATOM 10 NE ARG 1622 13 6.656 1.488 0.5	
2300 CZ APG 2300 6 300 6	
1301 NH1 APC 11.606 5.577	-+.70
1304 NH2 3DG 10.801 5 137	
1307 C 700	10.20
1308 0 370 15.877 5.050 -1.23 0.50	8.63
ATOM 1300 . ARG 1622 16 787 5.379 1.00	24.37
ATOM 1311 C ASP 1623 15.555 5.268 1.00	25.17
ATOM 10 102 1623 10 00 100 100 100 100	
ATOM - 15 22 CB ASP 1623 15 4.899 7.748 1 000	
ATOM CG ASP 1623 16 6.173 8.410 1.00	28.82
1314 ODI ACD 16./33 6 735	32.33
1315 OD2 ASD 16.276 7.520 10	36.67
1316 C 300 17.937 6 300	43.56
ATOM 1317 0 1623 16.408 3 766 9.463 1.00	36.29
ATOM 1318 N 1623 16.118 3 000 8.766 1.00	28.22
N LEU 1624 3.937 9.956 1.00	25 02
ATOM 1520 CA LEU 1624 15 2.592 8.278 1 00	26.87
ATOM 1524 LEU 1524 1624 9 132 1 22	26.34
1322 CG 1EU 16.996 0.169 1.00	26.59
1/, 082	24.59
SSSD/55145. v01	24.72

MOTA 1323 CD1 LEU 1624 15.844 -1.408 9.856 1.00 24.35 MOTA 1324 CD2 LEU 1624 17.258 -2.261 7.931 1.00 MOTA 1325 C LEU 1624 18.210 1.595 10.004 1.00 26.87 MOTA 1326 0 LEU 1624 19.322 1.777 9.497 1.00 28.19 ATOM 1327 N ALA 1625 18.009 1.570 11.317 1.00 27.77 MOTA 1329 CA ALA 1625 19.069 1.741 12.309 1.00 24.54 ATOM 1330 CB ALA 1625 19.355 3.210 12.494 1.00 19.81 MOTA 1331 С ALA 1625 18.498 1.173 13.592 1.00 26.44 MOTA 1332 0 ALA 1625 17.289 0.961 13.679 1.00 27.58 MOTA 1333 N ALA 1626 19.342 0.940 25.38 14.594 1.00 MOTA 1335 CA ALA 1626 18.872 0.397 15.865 1.00 24.65 MOTA 1336 CB ALA 1626 20.054 0.023 16.774 1.00 23.35 ATOM 1337 С ALA 1626 17.929 1.373 16.578 1.00 25.54 MOTA 1338 0 ALA 1626 17.057 0.951 17.325 1.00 27.70 ATOM 1339 N ARG 1627 2.671 18.104 16.344 1.00 25.06 ATOM 1341 CA ARG 1627 17.242 3.675 16.959 1.00 25.48 MOTA 1342 CB ARG 1627 17.706 5.089 16.597 1.00 28.15 MOTA 1343 CG ARG 1627 17.759 5.370 15.084 1.00 33.13 ATOM 1344 CD ARG 1627 18.157 6.811 14.774 1.00 33.29 MOTA 1345 NE ARG 1627 18.442 7.011 13.351 1.00 35.74 MOTA 1347 CZARG 1627 19.652 6.889 1.00 . 37.40 12.813 ATOM 1348 NH1 ARG 1627 20.695 6.585 13.575 1.00 39.73 **ATOM** 1351 NH2 ARG 1627 19.817 7.012 11.507 1.00 36.90 MOTA 1354 С ARG 1627 15.812 3.491 16.479 1.00 24.81 **ATOM** 1355 0 ARG 1627 14.871 3.853 17.173 1.00 24.05 MOTA 1356 N ASN 1628 15.667 2.910 15.293 1.00 24.80 MOTA 1358 ÇA ASN 1628 14.368 2.686 14.685 1.00 25.97 MOTA 1359 CB ASN 1628 14.383 3.132 13.225 1.00 30.08 **ATOM** 1360 CG 4.640 ASN 1628 14.417 13.096 1.00 33.62 MOTA 1361 OD1 ASN 1628 13.775 5.347 13.864 1.00 35.11 MOTA ND2 1362 ASN 1628 15.212 5.141 12.169 1.00 36.31 MOTA 1365 С ASN 1628 13.802 1.288 14.824 1.00 26.03 ATOM 1366 0 ASN 1628 12.951 0.869 14.031 1.00 26.87 MOTA 1367 N VAL 1629 14.330 0.550 15.797 1.00 26.04 MOTA 1369 CA VAL 1629 13.854 -0.783 16.128 1.00 25.09 MOTA 1370 CB VAL 1629 14.924 -1.876 15.959 1.00 27.00 ATOM 1371 CG1 VAL 1629 14.390 -3.197 16.546 1.00 20.99 MOTA 1372 CG2 VAL 1629 15.295 -2.051 14.462 1.00 23.26 MOTA 1373 C VAL 1629 13.504 -0.671 17.600 1.00 27.59 ATOM 1374 0 VAL 1629 14.340 -0.285 18.418 1.00 25.81 MOTA 1375 N LEU 1630 12.245 -0.929 17.923 1.00 28.17 ATOM 1377 CA LEU 1630 11.768 -0.845 19.296 1.00 30.20 ATOM 1378 CB LEU 1630 10.445 -0.077 19.332 1.00 30.26 ATOM 1379 CG LEU 1630 10.484 1.285 1.00 18.626 29.81 MOTA 1380 CD1 LEU 1630 9.119 1.983 18.745 1.00 28.46 MOTA 1381 CD2 LEU 1630 11.576 2.141 19.233 1.00 28.37 MOTA 1382 C LEU 1630 11.639 -2.242 19.904 1.00 29.32 MOTA 1383 0 LEU 1630 11.414 -3.219 19.189 1.00 30.84 **ATOM** 1384 N VAL 1631 11.800 -2.342 21.221 1.00 28.90 MOTA 1386 CA -3.629 VAL 1631 11.732 21.905 1.00 26.84 MOTA 1387 CB VAL 1631 13.067 -3.919 22.670 1.00 28.88 MOTA 1388 CG1 VAL 1631 13.077 -5.341 23.236 1.00 21.54 ATOM 1389 CG2 VAL 1631 14.259 -3.699 21.744 1.00 24.30 MOTA 1390 C VAL 1631 10.561 -3.645 22.881 1.00 29.02

ATOM 1392 V N TRR 1632 9.733 -4.674 22.764 1.00 30.84 ATOM 1395 CB TRR 1632 9.733 -4.674 22.764 1.00 30.84 ATOM 1395 CB TRR 1632 7.488 5.685 22.912 1.00 31.45 ATOM 1398 CG TRR 1632 7.286 -7.064 22.910 1.00 30.86 ATOM 1398 CG TRR 1632 7.286 -7.064 22.910 1.00 30.86 ATOM 1398 CG TRR 1632 8.919 -5.493 24.943 1.00 32.66 ATOM 1399 CG TRR 1632 8.919 -5.493 24.943 1.00 34.17 ATOM 1401 N GLU 1633 7.959 -5.524 25.866 1.00 36.16 ATOM 1404 CB GLU 1633 6.855 -6.163 27.177 1.00 36.16 ATOM 1404 CB GLU 1633 6.855 -6.163 27.177 1.00 36.16 ATOM 1404 CB GLU 1633 6.855 -6.063 27.996 1.00 37.07 ATOM 1406 CD GLU 1633 6.855 -6.063 27.996 1.00 37.07 ATOM 1408 OE2 GLU 1633 8.105 -6.000 30.301 1.00 49.38 ATOM 1409 OE2 GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1409 OE2 GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.952 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788 6.750 30.962 1.00 51.63 ATOM 1410 C GLU 1633 8.788	1	ATOM :	1391	0	1777								
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ATOM 1447 O MET 1637 10.480 -6.929 16.303 1.00 24.77  ATOM 1448 N LYS 1638 10.755 -4.791 16.931 1.00 25.74  ATOM 1451 CB LYS 1638 9.746 -4.258 16.029 1.00 23.67  ATOM 1452 CG LYS 1638 8.486 -3.888 16.799 1.00 21.78  ATOM 1453 CD LYS 1638 7.715 -5.092 17.298 1.00 24.60  ATOM 1454 CE LYS 1638 6.406 -4.683 18.005 1.00 23.87  ATOM 1454 CE LYS 1638 5.486 -5.897 18.256 1.00 23.06			С	MET		1	1.040			20.689		00 27	
ATOM 1448 N LYS 1638 10.755 -4.791 16.931 1.00 24.50 ATOM 1450 CA LYS 1638 9.746 -4.258 16.029 1.00 25.74 ATOM 1451 CB LYS 1638 8.486 -3.888 16.799 1.00 23.67 ATOM 1452 CG LYS 1638 7.715 -5.092 17.298 1.00 24.60 ATOM 1453 CD LYS 1638 6.406 -4.683 18.005 1.00 23.87 ATOM 1454 CE LYS 1638 5.486 -5.897 18.256 1.00 23.06			0	MET	1637	1	0.480				1.0		
ATOM 1450 CA LYS 1638 9.746 -4.258 16.029 1.00 25.74  ATOM 1451 CB LYS 1638 8.486 -3.888 16.799 1.00 23.67  ATOM 1452 CG LYS 1638 7.715 -5.092 17.298 1.00 24.60  ATOM 1453 CD LYS 1638 6.406 -4.683 18.005 1.00 23.87  ATOM 1454 CE LYS 1638 5.486 -5.897 18.256 1.00 23.06			N	LYS								0 24	
ATOM 1451 CB LYS 1638 8.486 -3.888 16.029 1.00 23.67  ATOM 1452 CG LYS 1638 7.715 -5.092 17.298 1.00 24.60  ATOM 1453 CD LYS 1638 6.406 -4.683 18.005 1.00 23.87  ATOM 1454 CE LYS 1638 5.486 -5.897 18.256 1.00 23.06				LYS							1.0		
ATOM 1452 CG LYS 1638 7.715 -5.092 17.298 1.00 21.78 ATOM 1453 CD LYS 1638 6.406 -4.683 18.005 1.00 23.87 ATOM 1454 CE LYS 1638 5.486 -5.897 18.256 1.00 23.06			CB	LYS							1.0		
ATOM 1453 CD LYS 1638 6.406 -4.683 18.005 1.00 24.60 ATOM 1454 CE LYS 1638 5.486 -5.897 18.256 1.00 23.06			CG				_				1.0		
ATOM 1454 CE LYS 1638 5.486 -5.897 18.256 1.00 23.87			CD	LYS			_				1.0		
3.486 -5.897 18.256 1.00 23.06	MOTA	1454	CE				_				1.0		
	cccn/e-				_	-	100	-5.	897	18.256	1.0		

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ATOM	1455	NZ	LYS	1638	4.871	-6.398	16.976	1.00	24.60
ATOM	1459	C	LYS	1638	10.260	-3.042	15.293	1.00	24.37
MOTA	1460	0	LYS	1638	10.658	-2.055	15.901	1.00	26.58
ATOM	1461	N	ILE	1639	10.271	-3.119	13.971	1.00	25.69
ATOM	1463	CA	ILE	1639	10.721	-2.005	13.148	1.00	25.94
MOTA	1464	CB	ILE	1639	10.935	-2.447	11.668	1.00	26.49
ATOM	1465	CG2	ILE	1639	11.218	-1.236	10.762	1.00	21.19
ATOM	1466	CG1	ILE	1639	12.103	-3.433	11.604	1.00	27.58
MOTA	1467	CD1	ILE	1639	12.120	-4.232	10.355	1.00	32.96
ATOM	1468	C	ILE	1639	9.675	-0.892	13.242	1.00	27.32
ATOM	1469	0	ILE	1639	8.466	-1.133	13.103	1.00	25.45
ATOM	1470	N	ALA	1640	10.156	0.320	13.498	1.00	27.43
ATOM	1472	CA	ALA	1640	9.321	1.499	13.632	1.00	26.96
ATOM	1473	CB	ALA	1640	9.557	2.133	15.006	1.00	25.21
MOTA	1474	C	ALA	1640	9.641	2.510	12.538	1.00	26.80
ATOM	1475	0	ALA	1640	10.691	2.446	11.896	1.00	27.55
ATOM	1476	N	ASP	1641	8.716	3.440	12.328	1.00	27.06
ATOM	1478	CA	ASP	1641	8.862	4.526	11.349	1.00	30.54
ATOM	1479	CB	ASP	1641	9.993	5.484	11.753	1.00	33.12
ATOM	1480	CG	ASP	1641	9.668	6.310	12.999	1.00	36.17
ATOM	1481	OD1	ASP	1641	10.477	7.203	13.334	1.00	42.24
ATOM ATOM	1482 1483	OD2 C	ASP	1641	8.633	6.076	13.648	1.00	33.22
ATOM	1484	0	ASP	1641	9.049	4.107	9.898	1.00	29.94
ATOM	1485	N	ASP PHE	1641	9.598	4.861	9.102	1.00	30.13
ATOM	1487	CA	PHE	1642 1642	8.569	2.920	9.553	1.00	30.22
ATOM	1488	CB	PHE	1642	8.680 8.462	2.426	8.191	1.00	30.91
ATOM	1489	CG	PHE	1642	7.156	0.909 0.470	8.159 8.750	1.00	26.24
ATOM	1490	CD1	PHE	1642	5.986	0.475	7.988	1.00	27.82 27.08
ATOM	1491	CD2	PHE	1642	7.089	0.026	10.066	1.00	26.70
ATOM	1492	CE1	PHE	1642	4.761	0.088	8.532	1.00	25.78
ATOM	1493	CE2	PHE	1642	5.872	-0.383	10.624	1.00	27.59
ATOM	1494	·CZ	PHE	1642	4.705	-0.354	9.855	1.00	28.05
MOTA	1495	С	PHE	1642	7.729	3.139	7.219	1.00	33.35
ATOM	1496	0	PHE	1642	7.983	3.165	6.018	1.00	36.19
ATOM	1497	N	GLY	1643	6.661	3.746	7.736	1.00	32.76
ATOM	1499	CA	GLY	1643	5.710	4.419	6.863	1.00	31.44
ATOM	1500	С	GLY	1643	5.805	5.927	6.910	1.00	32.94
MOTA	1501	0	GLY	1643	4.945	6.636	6.399	1.00	33.10
ATOM	1502	N	LEU	1644	6.872	6.407	7.525	1.00	35.45
MOTA	1504	CA	LEU	1644	7.124	7.828	7.684	1.00	39.04
ATOM	1505	CB	LEU	1644	8.387	8.011	8.514	1.00	37.80
ATOM	1506	CG	LEU	1644	8.414	9.120	9.549	1.00	42.51
ATOM	1507	CD1	LEU	1644	7.301	8.887	10.563	1.00	44.08
ATOM	1508	CD2	LEU	1644	9.779	9.127	10.243	1.00	44.47
MOTA	1509	C	LEU	1644	7.259	8.580	6.357	1.00	42.20
MOTA MOTA	1510	0	LEU	1644	7.895	8.107	5.414	1.00	44.14
	1511	N	ALA	1645	6.607	9.732	6.267	1.00	43.89
ATOM ATOM	1513	CA	ALA	1645	6.677	10.569	5.082	1.00	45.62
ATOM	1514	CB	ALA	1645	5.463	11.493	5.028	1.00	45.06
ATOM	1515 1516	C	ALA	1645	7.966	11.388	5.186	1.00	45.82
ATOM	1516	N O	ALA	1645	8.240	11.994	6.228	1.00	45.85
ATOM	1517	CA	ARG	1646	8.766	11.389	4.129	1.00	45.16
	<b></b>	CA	ARG	1646	10.015	12.140	4.138	1.00	47.06

	ATOM	1520	CB	ARG	3545						
	ATOM	1521	C		1646		126	11.318	4 7	0.4	
	ATOM .	1522	o	ARG	1646	10.4		12.546	4.7	`	-0.00
	ATOM	1523		ARG	1646	10.4		11.729	2.74		00 46.83
	3	1525	N	ASP	1647	10.8		12 024	1.82		00 45.76
			CA	ASP	1647	11.2		13.814	2.57	78 1.0	00 48.96
	7000	1526	CB	ASP	1647		_	4.291	1.28		-0.70
	<b>3</b>	1527	CG	ASP	1647	10.9		.5.769	1.07		-0.73
	ATOM	1528	OD1		1647	11.1	91 1	6.228	-0.36		
	ATOM :	1529	OD2			12.2	31 1	5.850	-0.95	_	
1	ATOM 1	1530	C		1647	10.3	40 1	6.980		_ `	50
		1531			1647	12.78		4.104	-0.89	_	
	_	.532	0		1647	13.49			1.336	5 1.00	50.78
			N	ILE	1648	13.27		4.803	2.077		48.32
			CA		1648	14.69	_	3.144	0.556	1.00	
	<b></b>		CB		648		_	2.833	0.516		
	TOM 1	536	~~~		648	14.98	4 11	.571	-0.324		
	TOM 1	537	~~			14.20	4 10	.386	0.241	•	
	TOM 1		<b>~</b>	_	648	14.63	8 11		-1.801		
A		539	~		648	15.23	3 10			1.00	48.22
A		`			648	15.523			-2.754	1.00	42.86
			-	LE 1	548	16.648		. 399	-0.018	1.00	55.57
		41 N	л н		549	14.944		. 222	0.423	1.00	57.24
			A H		49			766 .	0.936	1.00	
AT		-	B H		49	15.650		895 .	1.520	1.00	56.80
AT		45 C	_		49	15.013	16.	302 -	2.859		58.03
AT		46 C				15.221	15.		3.958	1.00	58.71
ATO	OM 154		D1 H			16:303	14.		4.306	1.00	60.28
ATO						14.241	14.			1.00	60.74
ATC					49	14.708	14.		4.874	1.00	61.70
ATO			22 HI	S 16	49	15.959	12.		5.742	1.00	61.86
ATO			HI	S 164	19	15.721	13.		5.417	1.00	60.98
ATO			HI	S 164	19	16 720	17.0	093 - (	0.591	1.00	
	-		HI		-	16.129	18.]	l75 - j	.004	1.00	58.49
ATO						5.285	16.9	916 c	.654		60.56
ATO		7 CB				5.306	18.0		.635	1.00	59.58
ATO	M 1558				_	3.898	18.5		.863	1.00	61.38
ATON	M 1559		-		_	3.404	19.4	_	700	1.00	65.28
ATON	1 1560				0 1	3.492	20.7		_	1.00	72.62
ATOM						2.710	18.9	_	. 536	1.00	76.23
ATOM				165		2.402	10.5	_	.339	1.00	77.05
ATOM			HIS	1650	) 7.	2.863	19.90	07 -1	157		78.51
	-505		HIS			003	21.01	L5 -0.	_		
ATOM		0	HIS	1650		925	17.57	<sup>75</sup> 2.			78.82
ATOM		N	ILE	1651		796	18.27		~ ~ ~		50.63
ATOM		CA	ILE			. 584	16.41				0.20
ATOM	1570	СВ		1651		.197	15.92	0 4			0.22
ATOM	1571		ILE	1651	17	.574	14.43			.00 6	0.03
ATOM	1572	CG2	ILE	1651	18	.280	13.92		069 1	.00 6	2.54
ATOM		CG1	ILE	1651	16	.329	13.52		323 1		3.48
	1573	CD1	ILE	1651	16	.635	13.58	4 3.1	300 1	.00 6	5.18
ATOM	1574	C	ILE	1651	10	. 635	12.124	4 3.6			
ATOM	1575	0	ILE		18	. 457	16.698	3 4.5			7.18
MOTA	1576	N	ASP	1651	19.	.326	16.907	3.7			9.16
ATOM	1578	CA		1652		532	17.176	-			9.25
ATOM	1579	CB	ASP	1652			17.915			00 58	3.91
ATOM	1580		ASP	1652		_	18 200			00 58	1.25
ATOM		CG	ASP	1652	20.		18.788			00 61	.14
ATOM	1581	OD1	ASP	1652	21.	<b>-</b> .	19.569		28 1.		.33
	1582	OD2	ASP	1652	20		19.574	7.4			
ATOM	1583	С	ASP	1652	20.		20.191	9.1			.11
			L	1002	20.	786 ;	16.922	6.6			.04
SSSD/55	145, vn1							J. 0	/6 1.0	JO 56	. 75



ATOM	1584	0	ASP	1652	20.699	16.307	7.741	1.00	56.06
MOTA	1585	N	TYR	1653	21.794	16.762	5.826	1.00	55.40
MOTA	1587	CA	TYR	1653	22.900	15.849	6.088	1.00	54.50
ATOM	1588	CB	TYR	1653	23.825	15.783	4.872	1.00	52.80
MOTA	1589	CG	TYR	1653	23.334	14.854	3.796	1.00	52.10
MOTA	1590	CD1	TYR	1653	24.123	14.566	2.685	1.00	51.50
ATOM	1591	CE1	TYR	1653	23.701	13.658	1.724	1.00	53.52
MOTA	1592	CD2	TYR	1653	22.099	14.214	3.917	1.00	52.88
ATOM	1593	CE2	TYR	1653	21.664	13.302	2.966	1.00	54.63
MOTA	1594	CZ	TYR	1653	22.469	13.025	1.870	1.00	54.35
MOTA	1595	OH	TYR	1653	22.049	12.107	0.933	1.00	53.23
ATOM	1597	С	TYR	1653	23.717	16.158	7.339	1.00	55.40
MOTA	1598	0	TYR	<b>16</b> 53	24.381	15.284	7.900	1.00	54.47
MOTA	1599	N	TYR	1654	23.673	17.409	7.773	1.00	56.72
MOTA	1601	CA	TYR	1654	24.421	17.826	8.947	1.00	58.87
ATOM	1602	CB	TYR	1654	24.978	19.235	8.733	1.00	57.91
ATOM	1603	CG	TYR	1654	26.068	19.269	7.685	1.00	60.49
ATOM	1604	CD1	TYR	1654	25.760	19.301	6.325	1.00	61.37
MOTA	1605	CE1	TYR	1654	26.769	19.289	5.356	1.00	63.72
MOTA	1606	CD2	TYR	1654	27.412	19.227	8.053	1.00	61.74
ATOM	1607	CE2	TYR	1654	28.425	19.216	7.099	1.00	64.08
MOTA	1608	CZ	TYR	1654	28.102	19.248	5.753	1.00	65.12
MOTA	1609	OH	TYR	1654	29. <b>1</b> 17	19.248	4.817	1.00	64.17
MOTA	1611	С	TYR	1654	23.628	17.732	10.245	1.00	60.17
ATOM	1612	0	TYR	1654	24.173	17.935	11.335	1.00	61.09
ATOM	1613	N	LYS	1655	22.348	17.393	10.133	1.00	60.54
MOTA	1615	CA	LYS	1655	21.493	17.277	11.306	1.00	62.12
ATOM	1616	CB	LYS	1655	20.019	17.382	10.910	1.00	64.32
MOTA	1617	CG	LYS	1655	19.054	17.346	12.079	1.00	67.17
ATOM	1618	CD	LYS	1655	17.644	17.608	11.602	1.00	73.05
ATOM	1619	CE	LYS	1655	16.626	17.243	12.660	1.00	77.36
ATOM	1620	NZ	LYS	1655	15.230	17.494	12.186	1.00	81.10
ATOM	1624	C	LYS	1655	21.754	15.976	12.057	1.00	62.19
ATOM	1625	0	LYS	1655	21.902	14.907	11.454	1.00	61.36
ATOM	1626	N	LYS	1656	21.822	16.084	13.380	1.00	62.26
ATOM ATOM	1628	CA	LYS	1656	22.069	14.933	14.236	1.00	62.28
ATOM	1629 1630	CB	LYS	1656	23.027	15.310	15.372	1.00	62.05
ATOM	1631	CD	LYS LYS	1656	24.474	15.489	14.957	1.00	62.62
ATOM	1632	CE	LYS	1656 1656	25.320	15.889	16.157	1.00	66.45
ATOM	1633	NZ	LYS	1656	26.803 27.619	15.666	15.908	1.00	67.28
ATOM	1637	C	LYS	1656		16.007	17.109	1.00	68.45
ATOM	1638	0	LYS	1656	20.774 19.714	14.381 15.007	14.824	1.00	61.86
ATOM	1639	N	THR	1657	20.875		14.733	1.00	62.95
ATOM	1641	CA	THR	1657	19.743	13.198	15.420	1.00	60.10
ATOM	1642	CB	THR	1657		12.541	16.053	1.00	57.73
ATOM	1643	OG1	THR	1657	19.973	11.012	16.121	1.00	56.04
ATOM	1645	CG2	THR	1657	21.150 20.152	10.730	16.896	1.00	55.21
ATOM	1646	C	THR	1657		10.431	14.731	1.00	53.07
ATOM	1647	0	THR	1657	19.664	13.102	17.472	1.00	57.74
ATOM	1648	N	THR	1658	20.513	13.899	17.870	1.00	57.76
ATOM	1650	CA	THR	1658	18.678 18.548	12.667	18.249	1.00	58.80
ATOM	1651	CB	THR	1658	17.318	13.140 12.517	19.627	1.00	60.33
ATOM	1652	C	THR	1658	19.811		20.290	1.00	61.37
	- 4 3 2	_	T 711/	TO 20	19.011	12.779	20.406	1.00	60.43

	ATOM	1653	0										
	ATOM	1654	N		1658	20.3	50	13.	599	21.			
	ATOM	1656			659	20.3	11		567	21.1		1.00	60.59
		1657	CA		659	21.5	08	11.	050	20.1	.61	1.00	59.97
	3	1658	CB		659	21.6			545	20.8		1.00	58.28
		1659	CG		659	22.4			883	20.6		1.00	59.95
		1660	OD1		659	22.3	82	9 -	265	21.7		1.00	60.10
		1663	ND2		659	23.2	10		367	22.8	91	1.00	61.26
		1664	_		559	22.78	31	11.7		21.3		1.00	57.09
					559	23.86	8	11.4		20.3		1.00	57.13
					60	22.64	3	12.5		20.79		1.00	57.34
			_		60	23.78	1			19.29		1.00	56.48
	<b>-</b>		_		60	24.53		13.2		18.73		1.00	54.87
				3LY 16	60	25.71		12.5		17.62		00	53.04
				\RG 16	61	23.87	9	12.8		17.39		.00	54.11
				RG 16	61	24.53		11.69		.6. <b>9</b> 1		.00	51.37
				RG 16	51	24.28	3	10.93		5.83		.00	48.96
				RG 166	51	24.848		9.42		5.96	1 1	.00	48.48
				RG 166	51	24.492		8.79		7.215	5 1	.00	50.03
AT				RG 166		25.013	•	7.32		7.234	1 1.		50.78
AT				RG 166		24.902		6.61		8.396	1.		50.11
AT		`		RG 166		24.286		5.29		3.566			50.08
ATO			Н2 ДІ	≀G 166	1	25.426		4.56		7.645	1.		46.57
ATO			A.	≀G 166		24.076		4.71		643	1.		17.88
ATO			AF	G 166		23.031		1.42		.459	l.		16.53
ATC			LE	TU 166		24.839		2.029		.325	ı.		5.01
ATO		<b></b>				24.546		1.094		.432	1.	00 4	2.39
ATO						25.823		1.503		.076	1.0		0.71
ATO						26.408		2.031		.399	1.0		0.25
ATO						27.853		3.332		. 965	1.0	00 4	2.44
ATO	_		2 LE	J 1662		25.591	13	3.478		. 537	1.0		0.42
ATO		_	LE			23.946		536		514	1.0		1.16
ATOM		_	LE	1662		24.647		.362		258	1.0		3.45
ATOM	_		PRO			22.632		.436		862	1.0		5.67
ATOM	_		PRO	1663	2	21.717		.428		987	1.0		7.09
ATOM			PRO		2	1.894		-475		489	1.0		.18
ATOM			PRO			0.535		.424		207	1.0		.59
ATOM		-	PRO	1663		0.343	10	098		983	1.00	_	. 90
ATOM	01	_	PRO	1663		2.556		. 856	11.	258	1.00	_	.13
ATOM	02	_	PRO	1663	2	2.362		045		376	1.00	33	.05
ATOM	-/03	N	VAL	1664		3.333		933		378	1.00		.16
ATOM		CA	VAL	1664	24	4.020		960	8.2	299	1.00		. 07
MOTA	1706	CB	VAL	1664	24	1.831		669	7.0		1.00		
ATOM	1707	CG1	VAL	1664	27	3.898		886	6.4	77	1.00		
	1708	CG2	VAL	1664	25	6.670		906	5.8		1.00		25
ATOM	1709	С	VAL	1664	24	0.070	11.		7.5		1.00		
ATOM	1710	0	VAL	1664	2.5	. 957		469	7.1	_	1.00	29.	
ATOM	1711	N	LYS	1665	25	.328		964	6.1		1.00	27.	
ATOM	1713	CA	LYS	1665	25	303		116	8.4		1.00	28.	
ATOM	1714	CB	LYS	1665	26	.189	6.9		8.6		00	27.	
ATOM	1715	CG	LYS	1665	26	.815	7.1		10.06		00	26.	
ATOM	1716	CD	LYS	1665		.967	8.0	89	10.07	`	.00	29.2	
ATOM	1717	CE	LYS	1665		. 283	8.6	19	11.46		.00		
ATOM	1718	NZ	LYS	1665	29.	. 543	9.4	78 .	11.42		.00	30.6	
ATOM	1722	С	LYS	1665	29.	826	10.1	28 ;	12.73		.00	30.9	
				±002	25.	546	5.6		8.46		.00	31.6	
SSSD/55	145 401									- 1	. 00	26.7	6

MOTA		0	LYS	1665	26.211	4.615	8.589	1.00	26.78
ATOM	1724	N	TRP	1666	24.260	5.630	8.137	1.00	25.79
ATOM	1726	CA	TRP	1666	23.561	4.381	7.865	1.00	26.56
ATOM	1727	CB	TRP	1666	22.299	4.273	8.724	1.00	25.63
ATOM	1728	CG	TRP	1666	22.564	3.872	10.174	1.00	26.95
ATOM	1729	CD2	TRP	1666	23.052	4.717	11.232	1.00	24.83
ATOM	1730	CE2	TRP	1666	23.134	3.920	12.398	1.00	24.49
MOTA	1731	CE3	TRP	1666	23.433	6.062	11.306	1.00	24.54
MOTA	1732	CD1	TRP	1666	22.376	2.636	10.730	1.00	20.10
MOTA	1733	NEl	TRP	1666	22.716	2.660	12.063	1.00	21.86
MOTA	1735	CZ2	TRP	1666	23.575	4.433	13.627	1.00	25.71
MOTA	1736	CZ3	TRP	1666	23.870	6.569	12.523	1.00	26.00
ATOM	1737	CH2	TRP	1666	23.939	5.754	13.665	1.00	26.04
ATOM	1738	C	TRP	1666	23.188	4.263	6.386	1.00	23.62
MOTA	1739	0	TRP	1666	22.754	3.214	5.931	1.00	24.87
MOTA	1740	N	MET	1667	23.404	5.330	5.631	1.00	22.78
MOTA	1742	CA	MET	1667	23.046	5.361	4.215	1.00	23.73
ATOM	1743	CB	MET	1667	22.894	6.802	3.744	1.00	26.24
MOTA	1744	CG	MET	1667	21.823	7.621	4.434	1.00	35.55
MOTA	1745	SD	MET	1667	21.795	9.276	3.706	1.00	42.23
ATOM	1746	CE	MET	1667	21.019	8.904	2.238	1.00	40.57
MOTA	1747	С	MET	1667	23.991	4.693	3.239	1.00	22.77
ATOM	1748	0	MET	1667	25.205	4.894	3.294	1.00	24.25
ATOM	1749	N	ALA	1668	23.420	3.963	2.286	1.00	22.73
ATOM	1751	CA	ALA	1668	24.217	3.337	1.237	1.00	23.54
ATOM	1752	CB	ALA	1668	23.339	2.495	0.340	1.00	21.80
ATOM	1753	C	ALA	1668	24.805	4.495	0.430	1.00	25.53
MOTA	1754	0	ALA	1668	24.181	5.551	0.316	1.00	23.66
MOTA	1755	N	PRO	1669	26.006	4.314	-0.153	1.00	26.86
ATOM	1756	CD	PRO	1669	26.899	3.144	-0.095	1.00	26.35
ATOM	1757	CA	PRO	1669	26.611	5.390	-0.942	1.00	27.78
ATOM	1758	CB	PRO	1669	27.864	4.731	-1.518	1.00	25.51
ATOM	1759	CG	PRO	1669	28.225	3.741	-0.471	1.00	25.36
ATOM	1760	С	PRO	1669	25.686	5.900	-2.057	1.00	26.47
ATOM	1761	0	PRO	1669	25.617	7.099	-2.288	1.00	28.42
ATOM	1762	N	GLU	1670	24:951	5.010	-2.724	1.00	26.88
ATOM	1764	CA	GLU	1670	24.057	5.459	-3.796	1.00	29.03
ATOM	1765	CB	GLU	1670	23.597	4.293	-4.693	1.00	31.79
ATOM	1766	CG	GLU	1670	22.588	3.325	-4.065	1.00	32.47
ATOM	1767	CD	GLU	1670	23.212	2.184	-3.255	1.00	32.43
MOTA	1768	OE1	GLU	1670	22.429	1.297	-2.822	1.00	25.01
ATOM	1769	OE2	GLU	1670	24.458	2.157	-3.069	1.00	28.75
ATOM	1770	С	GLU	1670	22.864	6.274	-3.294	1.00	28.37
ATOM	1771	0	GLU	1670	22.358	7.146	-4.001	1.00	25.72
ATOM	1772	N	ALA	1671	22.451	6.028	-2.053	1.00	30.08
ATOM	1774	CA	ALA	1671	21.347	6.779	-1.465	1.00	31.24
ATOM	1775	CB	ALA	1671	20.751	6.031	-0.287	1.00	26.42
ATOM	1776	C	ALA	1671	21.899	8.125	-1.013	1.00	31.36
ATOM	1777	0	ALA	1671	21.298	9.167	-1.249	1.00	33.11
ATOM	1778	N	LEU	1672	23.068	8.096	-0.387	1.00	32.73
ATOM	1780	CA	LEU	1672	23.715	9.304	0.100	1.00	33.96
ATOM	1781	СВ	LEU	1672	24.931	8.935	0.940	1.00	33.89
ATOM	1782	CG	LEU	1672	25.783	10.071	1.502	1.00	37.62
ATOM	1783	CD1	LEU	1672	25.010	10.800	2.581	1.00	39.57



TA	'OM	17	84 (	CD2 I	EU :	1672	27.05	4				
AT	MO	17	85 (	_		672	24.15			.087		0 32.30
AT	MO	178	86 C			672	23.769			.042		
AT	OM	178	37 N			673	24.959			.102	1.0	0 37.87
AT	MO	178	39 C			673	25.466			. 954	1.00	35.82
AT	MC	179	90 C		_	673		_		071	1.00	
AT(	MC	179	1 C	_		673	26.738			639	1.00	
ATC	MC	179	2 C	_		673	27.850	-		634	1.00	
ATO	MC	179	3 C			673	28.503			494	1.00	32.65
ATC	M	179	4 C			673	28.242 29.540	_		827	1.00	36.98
ATC		179	5 CI		_	573	29.279		•	555	1.00	37.95
ATO	M	179	6 C2		. –	573	29.279			881	1.00	39.90
ATO		179	7 C	PH		73				748	1.00	37.09
ATO	M	179	в о	PH		73	24.483	10.69		210	1.00	
ATO		179	9 и	AS		74	24.430	11.78			1.00	37.18
ATO		180	L CA			74	23.705	9.67			1.00	38.22
ATO		1802	CB			74	22.780	9.77			1.00	38.51
ATO		1803	CG			74	23.008	8.59			1.00	40.34
ATO	√I	1804	OD			74	24.439	8.51			1.00	43.87
MOTA	I	1805	OD				25.092	9.57			1.00	42.79
ATON		1806	C	AS			24.906	7.376			1.00	47.94
MOTA		1807	0	ASI			21.298	9.853		60	1.00	40.21
ATOM	-	1808	N	ARC			20.457	9.872			1.00	39.07
ATOM	1 :	1810	CA	ARC			20.975	9.836		72	1.00	39.83
ATOM	1 ]	1811	CB	ARC			19.589	9.900		31	1.00	42.25
ATOM	ני	1812	CG	ARG			18.992 19.691	11.271			1.00	48.19
ATOM		1813	CD	ARG			19.462	12.420			1.00	59.20
MOTA	_	814	NE	ARG			20.079	13.729			1.00	67.81
ATOM	1	816	CZ	ARG			19.688	14.876			1.00	75.11
ATOM		817	NH1				18.680	16.136			1.00	78.74
ATOM	1	820	NH2				20.311	16.429	-4.34		1.00	79.91
ATOM	1	823	С	ARG			18.730	17.115	-2.89		1.00	81.24
ATOM	1	824	0	ARG	167		17.544	8.777	-4.22		1.00	39.00
ATOM	1	825	N	ILE	167		19.345	8.956	-4.48		1.00	39.71
ATOM	1	827	CA	ILE	167		18.636	7.624	-4.43		1.00	35.50
ATOM	1	828	CB	ILE	167		19.434	6.471	-4.95		1.00	33.51
MOTA		829	CG2	ILE	167		18.582	5.759	-6.03		1.00	34.59
ATOM	18	330	CG1	ILE	1676		19.848	4.678	-6.64		1.00	33.90
ATOM	18	331	CD1	ILE	1676		20.861	6.752 6.197	-7.12		00	37.60
ATOM		332	C	ILE	1676	5	18.390	5.501	-8.10			42.67
ATOM		333	0	ILE	1676		19.326	4.926	-3.80			30.94
ATOM	18	34	N	TYR	1677		17.124	5.351	-3.25			28.62
ATOM		36	CA	TYR	1677		16.724		-3.44			30.60
ATOM		37	CB	TYR	1677		15.781	4.467	-2.359			25.87
ATOM		38	CG	TYR	1677		16.483	5.197	-1.413			26.40
ATOM	18	39	CD1	TYR	1677		16.663	6.220	-0.555			27.67
ATOM	18	40	CE1	TYR	1677		17.269	7.533	-0.999			27.45
ATOM	18	41	CD2	TYR	1677		16.935	8.483	-0.191		.00 2	26.55
ATOM	18	42	CE2	TYR	1677		17.536	5.883	0.721		.00 2	24.58
ATOM	18	43	CZ	TYR	1677		L7.698	6.828	1.538			26.35
ATOM	184	44	OH	TYR	1677		18.270	8.122	1.080		.00 2	8.80
ATOM	184	46	C	TYR	1677		16.055	9.059	1.914			4.97
ATOM	184	17	0	TYR	1677		5.144	3.235	-2.911			2.70
ATOM	184	18	N	THR	1678		.6.477	3.335	-3.728		00 2	6.22
						_	/	2.076	-2.420	1.		1.83
CCCC												

						145					
•								-2.865	1.00	22.1	4
			THR	1678	15.9		0.791		1.00	23.9	
MOTA	1850	CA	THR		16.9	07 (	0.191	-3.928	1.00	27.4	
MOTA	1851	CB		1678	18.2	29	0.105	-3.373	1.00	24.9	
MOTA	1852	OG1	THR	1678	16.9	49	1.053	-5.188	1.00	22.7	
MOTA	1854	CG2	THR	1678	15.9	99 -	0.176	-1.692	1.00	23.3	
ATOM	1855	С	THR		16.4	27	0.170	-0.592		21.9	
MOTA	1856	0	THR	1678	15.5	563 -	1.402	-1.929	1.00	22.9	
ATOM	1857	N	HIS	1679	15.6	513 -	2.417	-0.888	1.00	22.0	
ATOM	1859	CA	HIS	1679	14.		-3.671	-1.351	1.00	25.4	
ATOM	1860	CB	HIS	1679	13.		-3.444	-1.621	1.00	26.	
ATOM	1861	CG	HIS	1679	12.		-3.611	-2.740	1.00		13
ATOM	1862	CD2	HIS	1679	12.	•	-2.954	-0.663	1.00		
MOTA	1863	ND1	HIS	1679	12.		-2.830	-1.178	1.00		
MOTA	1865	CEl	HIS	1679	11.	_	-3.221	-2.441	1.00		
		NE2	HIS	1679	11.		-2.719	-0.650	1.00		
MOTA		_	HIS	1679	17.		-3.074	0.459		21.	.69
MOTA		_	HIS	1679	17.	.511	-2.506	-1.697	1.00		. 38
ATOM			GLN	1680	17	. 895	-2.726	-1.658		22	.33
MOTA			GLN			.335		-3.058	_	0 22	.52
MOTA		•	GLN			.948	-2.594	-3.87		0 29	.15
MOTA			GLN			.895	-3.872	-4.99		0 33	.60
MOTA			GL			.865	-3.847			0 38	.43
<b>IOTA</b>					17	.819	-3.212			0 33	.44
OTA	M 187				19	.159	-4.542	_		0 22	.61
OTA	M 187		Z GL		20	.007	-1.740		_		2.00
ATO			GL		20	.943	-2.093				2.06
OTA			SE		լ 19	562	-0.490				3.41
OTA	M 188					0.184	0.47				0.06
OTA	M 188				_	9.886	1.92				2.90
ATC	M 188				_	8.503	2.16	6 -0.4		_	3.08
OTA						9.778	0.20	6 1.5	-		4.13
TA					_	0.528	0.53			00 2	3.19
TA		89 0			_	8.608	-0.41				2.37
ATO		90 N		SP 168	_	8.107	-0.77	5 3.1	-		4.55
TA		92 C		SP 168	_	6.660	-1.27	75 3.0	_		24.22
AT		93 C		SP 168		15.616	-0.1	72 3.2	-		25.02
		94 C	_	SP 168	_	14.428	-0.4	79 3.0			24.82
		95 0		SP 16		15.949	0.9	68 3.€			20.47
				SP 16		18.980	-1.8	88 3.0			21.83
		397 (	_	SP 16		19.172	-1.9	84 4-			
			o 1	ASP 16		19.480	-2.7	46 2.	_		20.14
			N '		-		-3.8	56 3.		.00	20.49
			CA	• • • • • • • • • • • • • • • • • • • •	83	20.340			003 1	00	22.38
				• • • • • • • • • • • • • • • • • • • •	83	20.493			159	1.00	19.57
				VAL 16	83	21.757			942	1.00	22.35
				VAL 1	583	19.264			683	1.00	20.22
A		.905	C		583	21.677		_	684	1.00	21.41
			0	VAL 1	683	22.202			. 003	1.00	21.33
		1906	N	• -	684	22.210	-2.	-		1.00	22.21
		1907	CA		684	23.440		-	.540	1.00	18.78
		1909			684	23.768			.037	1.00	22.80
·. 1		1910	CB	•	684	24.92	•	_	477	1.00	24.60
		1911	CG		.684	26.23	7 0.		.472	1.00	24.34
	MOTA	1912	CD2	••••	1684	26.98	9 1.		.286	1.00	24.32
	MOTA	1913	CE2		1684	26.85	3 -0		.352	1.00	22.28
	ATOM	1914	CE3	•••		24.93	3 1	.208 4	1.138	1.00	
	MOTA	1915	CD1	TRP	1684						

_			146			
ATOM 191	6 NE1 TRP	160.				
ATOM 191		1684 2	6.169	1.791	4 205	
ATOM 191		1684 2	8.324	1.669	4.297	1.00 22.32
ATOM 192		1684 28	3.193	0	3.022	1.00 24.77
ATOM 192:	TRE	1684 28		•	1.090	1.00 24.46
ATOM 1922		1684 23			1.918	1.00 24.00
ATOM 1923	IRP	1684 23			4.899	1.00 23.26
ATOM 1925	O. SEK	1685 22			5.805	1.00 24.52
ATOM 1926	SEK	1685 .21	~ .		5.113	1.00 22.88
ATOM 1927	CB SER	1685 20			.444	1.00 24.01
ATOM 1929	OG SER	1685 20		.783 6	.385	
Ame.	C SER		_	.787 <sub>5</sub>	_	_
A moss.	O SER	L685 22		.087 7		
Amo.	N PHE 1			.933 g		
	(°)		099 -2	.221 7	027	
	CB			.393 <sub>7.</sub>		23.20
ATOM 1935		-0.	216 -4.		_	23.87
ATOM 1936	CD1		062 <sub>-5</sub>	_		00 19.56
ATOM 1937			240 -5		_	.00 22.19
ATOM 1938	CE1	686 20.	773 -6	_	_	.00 21.55
ATOM 1939	CD2 - T6	586 19.1	-25 -6.			.00 21.94
ATOM 1940	TC	20.6	.63 -8.∂			.00 21.66
ATOM 1941	C 200-	<sup>86</sup> 19.8	42 -7 6			.00 22.47
ATOM 1942	V TP	86 22.3	289 - ק			00 23.14
ATOM 1943	M 02.12	<sup>86</sup> 22.5	79 -4.4			00 22.62
ATOM 104-	Cy 22	87 23.3:	54 -3.7	_		00 23.09
ATOM	~ 011 16	87 24.7			01 1.	00 23.50
ATOM TOLE	221 186	<sup>37</sup> 25.23	· -			00 23.83
<b>ΔΤΟΜ</b>	GLY 168	25.90			67 1.	
ATOM 1050	VAL 168	18 24.92		<sup>49</sup> 9.7	78 1.0	
ATOM 105	A VAL 168	8 25.33			17 1.0	
ATOM 1000	B VAL 168	8 25.02			77 1.0	
ATOM 1000	G1 VAL 168	8 25.54	_		38 1.0	
ATOM an-	G2 VAL 168			8 10.54	3 1.0	
Amore	VAL 168			2 8.16	0 1.0	
0	VAL 1688	~ =		0 11.18	2 1.0	-
	LEU 1689	-3.133	,	9 12.25	_	
ATOM 1958 C		40.510	-1.70	11.08	_	-2.70
ATOM 1959 CE	LEU 1689		-2.111			-2.01
ATOM 1960 CG		004	-2.357			
ATOM 1961 CD			-2.491			
ATOM 1962 CD	2 2 2009	-0.043	-2.109	12.408	•	
ATOM 1963 C	-20 1089	19.959	-3.895		_	,
ATOM 1964 O		23.158	-3.375			
ATOM 1965 N	LEU 1689	23.249	-3.483	12.871		25.88
ATOM 1967 CA	LEU 1690	23.588	-4.323	14.099		26.50
ATOM 1055	LEU 1690	24.221	-5 544	12.031	1.00	25.84
ATOM	LEU 1690	24.669	-5.544	12.523	1.00	24.43
ATOM 1000	LEU 1690	23.672	-6.444	11.377	1.00	26.35
ATOM TO	LEU 1690	24.415	-7.309	10.604	1.00	26.57
ATOM TO	LEU 1690	23.042	-7.962	9.446	1.00	26.37
ATOM	LEU 1690	25 420	-8.380	11.502	1.00	26.33
ATOM 3.5	LEU 1690	25.430	-5.168	13.349	1.00	24.66
ATOM 1974 N	TRP 1691	25.646	~5.706	14.435	1.00	25.22
ATOM 1976 CA	TRP 1691	26.211	~4.227	12.826		24.84
ATOM 1977 CB	TRP 1691	27.405	-3.728	13.504	1.00	26.92
ATOM 1978 CG		28.072	-2.659	12.631	1.00	25.77
	TRP 1691	29.394	-2.195		1.00	24.82
SSSD/55145. v01				13.154	1.00	27.98

MOTA 1979 CD2 26.95 TRP 1691 29.623 -1.104 14.056 1.00 MOTA 1980 CE2 TRP 1691 31.022 -1.015 14.259 1.00 27.64 MOTA 1981 CE3 TRP 1691 28.783 -0.191 14.708 1.00 ATOM 1982 CD1 TRP 1691 30.634 -2.715 12.856 1.00 28.38 **ATOM** 1983 NE1 TRP 1691 31.609 -2.009 13.518 1.00 29.56 **ATOM** 1985 CZ2 TRP 31.599 -0.045 1691 15.086 1.00 27.78 ATOM 1986 CZ3 TRP 0.769 1691 29.356 15.533 1.00 27.63 ATOM 1987 CH2 TRP 30.753 1691 0.835 15.713 1.00 30.68 ATOM 1988 С TRP 1691 27.025 -3.147 14.876 1.00 26.38 MOTA 1989 0 TRP 1691 27.686 -3.414 15.883 1.00 24.82 MOTA 1990 N GLU 1692 25.926 -2.393 14.916 1.00 27.62 MOTA 1992 CA GLU 1692 25.442 -1.790 16.162 1.00 27.02 MOTA 1993 CB GLU 1692 24.193 -0.963 15.919 1.00 29.27 ATOM 1994 CG GLU 24.345 1692 0.236 15.028 1.00 24.77 MOTA 1995 CD GLU 1692 23.046 0.992 14.962 1.00 25.98 ATOM 1996 OE1 GLU 1692 22.238 0.694 14.058 1.00 22.29 **ATOM** 1692 1997 OE2 GLU 22.803 1.837 15.850 1.00 25.12 ATOM 1998 C GLU 1692 25.092 -2.856 17.191 1.00 27.88 MOTA 1999 0 GLU 1692 25.333 -2.673 18.379 1.00 30.18 MOTA 2000 N ILE 1693 24.500 -3.956 16.734 1.00 26.65 MOTA 2002 CA ILE 1693 24.118 -5.054 17.618 1.00 26.14 **ATOM** 2003 CB ILE 1693 23.279 -6.144 16.858 1.00 25.37 MOTA 2004 CG2 ILE 1693 23.144 -7.445 17.704 1.00 21.48 MOTA 2005 CG1 ILE 1693 21.897 -5.563 16.496 1.00 24.80 MOTA 2006 CD1 ILE 1693 21.017 -6.479 15.642 1.00 22.40 ILE MOTA 2007 С 1693 25.345 -5.698 18.239 1.00 27.17 ATOM 2008 С ILE 1693 25.424 -5.864 19.452 1.00 27.30 MOTA 2009 N PHE 1694 26.329 -6.017 17.414 1.00 29.98 MOTA 2011 CA PHE 1694 27.518 -6.674 17.925 1.00 30.61 MOTA 2012 CB PHE 1694 -7.556 28.140 16.843 1.00 28.30 MOTA 2013 CG PHE 1694 27.197 -8.611 16.353 1.00 30.91 MOTA 2014 CD1 PHE 1694 26.627 -8.526 15.088 1.00 34.46 MOTA 1.00 2015 CD2 PHE 1694 -9.601 17.224 26.743 32.71 ATOM 2016 14.701 CE1 PHE 1694 25.622 -9.409 1.00 34.24 MOTA 2017 CE2 PHE 1694 25.737 -10.490 16.844 1.00 32.44 ATOM 2018 CZPHE 1694 25.170 -10.387 15.592 1.00 32.70 MOTA 2019 С PHE 1694 28.512 -5.796 18.689 1.00 31.74 ATOM 2020 0 PHE 1694 -6.299 29.469 19.276 1.00 35.15 MOTA 2021 N THR 1695 28.275 -4.489 18.698 1.00 31.12 ATOM 2023 CA THR 1695 29.101 -3.575 19.473 1.00 29.96 MOTA 2024 CB THR 1695 29.532 -2.351 18.657 1.00 28.09 MOTA 2025 OG1 THR 1695 28.373 -1.685 18.150 1.00 30.65 MOTA 2027 CG2 THR 1695 30.450 -2.767 17.510 1.00 23.37 MOTA 2028 С THR 1695 28.240 -3.128 20.664 1.00 30.01 MOTA 2029 -2.233 0 THR 1695 28.617 21.427 1.00 31.14 MOTA 2030 1.00 N LEU 1696 27.078 -3.766 20.797 27.96 MOTA 2032 CA LEU 1696 26.113 -3.490 21.862 1.00 30.25 MOTA 2033 CB LEU 1696 26.633 -3.985 23.216 1.00 33.54 MOTA 2034 CG LEU 1696 26.899 -5.482 23.339 1.00 32.61 MOTA 2035 CD1 LEU 1696 27.473 -5.777 24.711 1.00 33.54 MOTA 2036 CD2 LEU 1696 25.602 -6.233 23.126 1.00 36.37 MOTA 2037 С LEU 1696 25.717 -2.031 21.958 1.00 28.19 MOTA 2038 LEU 0 1696 25.792 -1.431 23.018 1.00 29.18 MOTA 2039 N GLY 1697 25.251 -1.472 20.853 1.00 28.24

							_				
	ATO		CA	GLY	1.500						
	ATO	M 2042			1697	24.	851	-0.082	20.858		
	ATO		-	GLY	1697	25.	990	0.845			-0.2)
	ATON		_	GLY	1697	25.	960	2.022		-	27.68
	ATOM			GLY	1698	26.	986	0.324	20.846	_	29.79
	ATOM		CA	GLY	1698	28.3		1.324	19.790	1.00	29.23
	ATOM		C ,	GLY	1698	27.7		1.143	19.396	1.00	30.79
	ATOM		0	~	1698	26.8		2.212	18.388	1.00	32.38
			N		1699	20.0	_	2.044	17.601	1.00	
	ATOM		CA	^	1699	28.4		3.314	18.411	1.00	33.26
	ATOM	2052	CB		.699	28.2	68	4.437	17.510	1.00	30.81
	ATOM	2053	OG			28.5	28	5.728	18.288		32.03
	ATOM	2055	C		699	28.5	59 (	5.862	17.440	1.00	34.81
	ATOM	2056	_	_	699	29.19	98 4	1.325	16.282	1.00	40.03
	ATOM	2057			699	30.42	28 4	.325		1.00	32.20
	ATOM	2058			700	28.62		.148	16.408	1.00	31.67
	ATOM	2059			700	27.17			15.082	1.00	32.62
	ATOM	2060		PRO 1	700	29.42	_	.142	14.773	1.00	34.19
	ATOM			PRO 17	700	28.35		.028	13.856	1.00	31.76
	ATOM	2061		-	700	27.14	_	.830	12.759	1.00	32.04
	ATOM	2062	C I		00	30 21		.351	13.502	_	
			0 p		00	30.21		. 309	13.609		33.17
	ATOM			YR 17		29.719		.391			28.70
	ATOM			YR 17		31.459	5.	181			28.57
	MOTA	2067				32.311	6.			1.00	28.61
	ATOM	222				31.920	6.				29.92
	ATOM	2000				31.965	5.			1.00 3	30.15
	ATOM	2020		(R 17)		30.799	5.			1.00 з	6.17
				_		30.839	4			00 з	9.26
					1	33.176			8.571 1		1.51
	70000		E2 TY		1 ;	33.229			9.893 1		7.48
	N MOL-		Z TY	R 170		32.059			8.805 1		2.94
	3000.			R 170		32.110	4.2	_	8.146 1		5.72
		076 C		R 170	1 3	2.279	3.4		7.043 1		3.99
		077 0	TY	R 170	1 7	1.935	7.4		n 4		1.09
	3	078 N	PRO		_	2.649	8.5				93
	7 moss	079 CI	PRO		_	2.049	7.1	35 15			
		080 CA	PRO			3.212	5.8	79 15			.66
	ATOM 2	081 CE			-	2.631	8.1	73 16	_		.83
		082 CG				3.116	7.43	32 17			. 54
	ATOM 20	083 C	PRO			2.903	6.00	17			.18
		)84 O	PRO			3.628	9.27			_	. 82
1	ATOM 20	85 ท			34	750	8.98				. 78
7		0.7	GLY	1703	33	.220	10.52	_			. 97
7	ATOM 20		GLY	1703	34	.085	11.66	-	074 1.0		45
	ATOM 20		GLY	1703	34	.245	12.00		788 1.0	0 34.	
A	TOM 20	• •	GLY	1703	34	. 977	12.00		317 1.0	0 34.	34
			VAL	1704	33	. 552	12.93		969 1.0	0 34.	
	<b>7701</b>		VAL	1704	33	.641	11.27		445 1.0		
			VAL	1704			11.512	2 12.	007 1.0		
	TOM 209		VAL	1704		. 614	10.176	11.3		_	
	TOM 209	5 CG2				.628	10.435	9.7	709 1.0		
	TOM 209		VAL	1704	34.	796	9.297				
A:	TOM 209	-		1704	32.	510	12.410				
A <sup>r</sup>	TOM 209	_	VAL	1704	31.	337	12.070			95.5	
AT	TOM 209	_	PRO	1705	32.		13.589				4
	TOM 210	_	PRO	1705	34.		14.221	_		32.4	
	OM 210		PRO	1705	31.		14.505	10.9	_	32.7	
	- 2101	l CB	PRO	1705	32.		15 00-	10.4	72 1.00	33.6	
SSC	SD/55145. v	•			_ •		15.853	10.5	09 1.00	33.2	
	· ・ ・	// 1 T								4.	-

MOTA 2102 CG PRO 1705 33.935 15.482 10.141 1.00 35.53 31.395 ATOM 2103 С PRO 1705 14.138 9.052 1.00 33.91 MOTA 2104 0 PRO 1705 32.113 13.409 1.00 8.354 32.65 **ATOM** 2105 N VAL 1706 30.255 14.684 8.619 1.00 33.82 ATOM 2107 CA VAL 1706 29.689 14.447 7.280 1.00 33.97 2108 MOTA CB VAL 1706 28.617 15.513 6.943 1.00 37.41 MOTA 2109 CG1 VAL 1706 28.045 15.282 5.556 1.00 41.12 MOTA 2110 CG2 VAL 1706 27.507 15.484 7.971 1.00 38.89 MOTA 2111 C VAL 30.712 1706 14.428 6.135 1.00 32.32 MOTA 2112 0 VAL 1706 30.819 13.450 5.398 1.00 32.58 MOTA 2113 N GLU 1707 31.477 15.504 6.004 1.00 31.15 ATOM 2115 CA GLU 32.478 15.630 4.956 1.00 1707 29.82 MOTA 2116 CB GLU 1707 33.172 16.989 5.048 1.00 30.05 14.541 MOTA 2117 С GLU 1707 33.531 4.959 1.00 28.52 MOTA 2118 GLU 0 1707 33.995 1.00 14.134 3.896 30.85 MOTA 2119 N GLU 1708 33.958 14.110 6.143 1.00 28.70 MOTA 2121 CA GLU 1708 34.978 13.073 6.235 1.00 29.50 MOTA 2122 CB GLU 7.641 1708 35.590 13.010 1.00 31.28 ATOM 2123 CG GLU 1708 36.281 14.289 8.103 1.00 41.63 ATOM 2124 CD GLU 1708 37.454 14.718 7.237 1.00 49.91 MOTA 2125 OE1 GLU 1708 38.020 13.876 6.498 1.00 53.57 MOTA 2126 OE2 GLU 1708 37.821 15.916 7.308 1.00 58.45 MOTA 2127 C GLU 1708 34.365 11.730 5.878 1.00 30.00 MOTA 2128 35.016 0 GLU 1708 10.874 5.257 1.00 28.43 MOTA 2129 N LEU 1709 33.103 11.559 6.257 1.00 30.08 CA ATOM 2131 LEU 1709 32.392 10.324 5.964 1.00 29.19 MOTA 2132 CB LEU 1709 30.995 10.347 6.592 1.00 28.97 MOTA 2133 CG LEU 1709 30.109 6.137 9.186 1.00 30.66 ATOM 2134 CD1 LEU 1709 30.664 7.866 6.659 1.00 29.24 MOTA CD2 2135 LEU 1709 28.684 9.403 6.593 1.00 29.29 MOTA 10.130 2136 C LEU 1709 32.294 4.449 1.00 28.26 ATOM 2137 LEU 0 1709 32.450 9.011 3.948 1.00 28.86 MOTA 2138 N PHE 1710 32.016 11.220 3.735 1.00 26.86 MOTA 2140 CA PHE 1710 31.903 11.192 2.285 1.00 28.86 MOTA 2141 CB PHE 1710 31.632 12.593 1.743 1.00 31.88 ATOM 2142 CG PHE 1710 30.249 13.095 2.014 1.00 37.62 MOTA 2143 CD1 PHE 1710 29.265 12.247 2.509 1.00 42.63 MOTA 2144 CD2 PHE 1710 29.931 14.424 1.792 1.00 43.53 MOTA 2145 CE1 PHE 1710 27.977 12.718 2.783 1.00 45.99 ATOM 2146 CE2 PHE 1710 28.648 14.905 2.061 1.00 46.25 ATOM 2147 CZPHE 1710 27.670 14.045 2.559 1.00 44.45 MOTA 2148 С PHE 1710 33.193 10.660 1.681 1.00 30.42 ATOM 2149 O . PHE 1710 33.174 9.807 0.792 1.00 29.01 MOTA 2150 N LYS 1711 34.309 2.212 1.00 11.152 30.64 MOTA 2152 CA LYS 1711 35.650 10.762 1.786 1.00 32.89 2153 CB ATOM LYS 1711 36.670 11.655 2.502 1.00 37.91 MOTA 2154 CG LYS 1711 38.108 11.479 2.088 1.00 42.99 **ATOM** 2155 CD LYS 1711 38.976 12.528 2.752 1.00 47.45 ATOM 2156 CE LYS 1711 40.380 12.505 2.182 1.00 52.35 MOTA 2157 NZ LYS 1711 41.104 11.272 2.587 1.00 58.47 ATOM 2161 С LYS 1711 35.913 9.273 2.071 1.00 32.23 ATOM 2162 0 LYS 1711 36.445 8.559 1.216 1.00 30.79 ATOM 2163 N LEU 1712 35.533 8.807 3.264 1.00 31.37 MOTA 2165 CA LEU 1712 35.704 7.399 3.630 1.00 29.46

A	TOM 2	2166	CD	• <b>-</b>					
		167				220 7.3	117 5.0	065 1.00	_
					'12 36.	045 7.6			
					12 35.	395 7.3			
			_		12 37.	452 7.0			
				EU 17	12 34.				90.00
			_	EU 17	12 35.4				
				EU 17					30.73
				EU 17					30.13
				EU 17:	13 31.4		-		32.10
		_		EU 173	13 30.6	-			35.23
		_		EU 171				-	37.47
AT	_			EU 171	.3 30.4				40.85
AT		79 C		EU 171					39.61
ATO		80 O	L	EU 171	3 33.5				32.70
ATO		•	LY	S 171	4 33.8				31.86
ATO			A Ly			•			32.42
ATO		84 C	B LY						32.56
ATO		85 C	3 LY		9				33.02
ATC		36 CI				•		7 1.00	35.56
ATC			LY		,-	•	_	6 1.00	37.94
ATO		88 N2			02			2 1.00	42.57
ATO		2 C	LY					9 1.00	47.40
ATO		3 0	LY					5 1.00	35.36
ATO		4 N	GL					7 1.00	36.68
ATO		6 CA							34.51
ATO!	M 219	7 CB					-0.749		35.31
ATO	M 219	8 CG							37.07
ATON		9 CD			38.96	• ,		1.00	43.62
ATOM		OE:			39.73		0.893		49.75
ATOM	1 220:	OE:			39.906		2.029	_	49.71
ATOM	2202	2 C	GLU		40.163		0.572		55.13
ATOM	2203	3 0	GLU		37.321		-0.487		34.08
ATOM	2204	N	GLY	1716	38.259		-0.438		34.82
ATOM	2206	CA	GLY	1716	36.049		~0.366		31.53
ATOM	,	C	GLY	1716	35.695	. – • •	-0.133		27.58
ATOM	2208		GLY	1716	35.966		1.262	_	88.60
ATOM	2209	N	HIS	1717	36.069		1.464		27.81
ATOM	2211	CA	HIS	1717	36.062	2.663	2.236		9.10
ATOM	2212	CB	HIS	1717	36.319	2.263	3.617		9.30
ATOM	2213	CG	HIS	1717	36.501	3.510	4.486		0.54
ATOM	2214	CD2	HIS	1717	36.788	3.213	5.930		2.88
ATOM	2215	ND1	HIS	1717	37.961	3.023	6.586		2.21
ATOM	2217	CE1	HIS	1717	35.798	3.108	6.881	_	4.22
ATOM	2218	NE2	HIS		36.342	2.865	8.061	_	1.51
ATOM	2220	C	HIS	1717	37.651	2.809	7.907		1.94
ATOM	2221	Ö	HIS	1717	35.180	1.416	4.183		
ATOM	2222	N		1717	34.017	1.666	3.885		3.42
ATOM	2224	CA	ARG	1718	35.526	0.450	5.028		7.71
ATOM	2225	CB	ARG	1718	34.559	-0.423	5.688		7.75
ATOM	2226	CG	ARG	1718	34.562	-1.813	5.048	•	.58
ATOM	2227	CD	ARG	1718	34.078	-1.860	3.597		.07
ATOM	2228		ARG	1718	32.609	-1.412	3.475		.39
ATOM	2230	NE CZ	ARG	1718	32.091	-1.467	2.096		. 64
ATOM	2231	CZ	ARG	1718	32.173	-0.476			.37
•••	~ C 3 T	NH1	ARG	1718	32.768	0.668			. 26
SSSD/SE	14501						4.332	1.00 23	. 98

2234	NH2	ARG	1718	31.595	-0.603	0.019	1.00	21.60
2237	С	ARG	1718	35.005	-0.521	7.148	1.00	30.11
2238	0	ARG	1718	36.201	-0.623	7.428	1.00	30.60
2239	N	MET	1719	34.056	-0.430	8.074	1.00	30.69
2241	CA	MET	1719	34.350	-0.490	9.501	1.00	31.77
2242	CB	MET	1719	33.072	-0.302	10.335	1.00	34.56
2243	CG	MET	1719	32.408	1.060	10.194	1.00	36.71
2244	SD	MET	1719	31.015	1.307	11.314	1.00	38.66
2245	CE	MET	1719	29.797	0.338	10.544	1.00	36. <b>9</b> 9
2246	С	MET	1719	34.998		9.854	1.00	30.20
2247	0	MET	1719	34.802	-2.802	9.169	1.00	31.41
2248	N	ASP	1720	35.778	-1.809	10.926		32.49
2250	CA	ASP	1720			11.385		33.60
2251	СВ	ASP						37.65
2252								44.69
								50.97
								48.67
								31.26
								32.69
								32.76
								32.28
								33.63
								35.68
								36.22
								42.65
								46.15
								35.55
								37.78
								36.91
								34.43
								37.77
2273								36.32
								34.53
								39.31
	0							38.78
	N							42.72
								45.01
								46.88
2281	OG							53.47
2283	С							46.67
2284	0							46.21
	N							47.80
								52.78
								57.86
								61.99
								63.17
								63.56
								51.43
								51.56
								48.91
								45.62
								44.83
								41.83
4 J U L		C12	1/23	34.341	-12.135	15.640	1.00	42.30
	2237 2238 2239 2241 2242 2243 2244 2245 2246 2247 2248 2250 2251 2252 2253 2254 2255 2256 2257 2260 2261 2262 2263 2264 2268 2269 2270 2271 2272 2273 2274 2275 2276 2277 2279 2280 2281	2237 C 2238 O 2239 N 2241 CA 2242 CB 2243 CG 2244 SD 2245 CE 2246 C 2247 O 2248 N 2250 CA 2251 CB 2252 CG 2253 OD1 2254 OD2 2255 C 2256 O 2257 N 2259 CA 2260 CB 2261 CG 2262 CD 2263 CE 2264 NZ 2268 C 2269 O 2270 N 2271 CD 2272 CA 2273 CB 2271 CD 2272 CA 2273 CB 2274 CG 2275 C 2276 O 2277 N 2279 CA 2271 CD 2272 CA 2273 CB 2274 CG 2275 C 2276 O 2277 N 2279 CA 2278 CB 2281 OG 2277 N 2279 CA 2288 CB 2281 OG 2281 OG 2281 OG 2281 OG 2281 OG 2283 C 2284 O 2285 N 2287 CA 2288 CB 2289 CB 2289 CG 2290 OD1 2291 ND2 2294 C 2295 O 2296 N 2298 CA 2298 CA 2299 CB 2300 SG	2237         C         ARG           2238         O         ARG           2239         N         MET           2241         CA         MET           2242         CB         MET           2243         CG         MET           2244         SD         MET           2245         CE         MET           2246         C         MET           2247         O         MET           2248         N         ASP           2250         CA         ASP           2251         CB         ASP           2252         CG         ASP           2253         OD1         ASP           2254         OD2         ASP           2255         C         ASP           2257         N         LYS           2259         CA         LYS           2260         CB         LYS           2261         CG         LYS           2262         CD         LYS           2263         CE         LYS           2264         NZ         LYS           2265         CD         LYS	2237         C         ARG         1718           2238         O         ARG         1718           2239         N         MET         1719           2241         CA         MET         1719           2242         CB         MET         1719           2243         CG         MET         1719           2244         SD         MET         1719           2245         CE         MET         1719           2246         C         MET         1719           2247         O         MET         1719           2248         N         ASP         1720           2250         CA         ASP         1720           2251         CB         ASP         1720           2251         CB         ASP         1720           2253         OD1         ASP         1720           2254         OD2         ASP         1720           2255         C         ASP         1720           2257         N         LYS         1721           2250         CA         LYS         1721           2261         CG         LYS	2237         C         ARG         1718         35.005           2238         O         ARG         1718         36.201           2239         N         MET         1719         34.056           2241         CA         MET         1719         34.350           2242         CB         MET         1719         32.408           2244         SD         MET         1719         32.408           2244         SD         MET         1719         34.998           2245         CE         MET         1719         34.998           2247         O         MET         1719         34.998           2247         O         MET         1719         34.998           2247         O         MET         1719         34.998           2248         N         ASP         1720         35.778           2250         CA         ASP         1720         36.473           2251         CB         ASP         1720         36.473           2252         CG         ASP         1720         38.442           2253         OD1         ASP         1720         35.524	2237         C         ARG         1718         35.005         -0.521           2238         O         ARG         1718         36.201         -0.623           2239         N         MET         1719         34.056         -0.430           2241         CA         MET         1719         33.072         -0.302           2243         CG         MET         1719         31.015         1.307           2244         SD         MET         1719         31.015         1.307           2245         CE         MET         1719         31.015         1.307           2245         CE         MET         1719         31.015         1.307           2245         CE         MET         1719         34.998         -1.810           2247         O         MET         1719         34.802         -2.802           2248         N         ASP         1720         35.778         -1.819           2250         CA         ASP         1720         38.628         -1.688           2251         CB         ASP         1720         38.628         -1.688           2253         OD1         ASP	2237         C         ARG         1718         35.005         -0.521         7.428           2238         N         ARG         1718         36.201         -0.623         7.428           2241         CA         MET         1719         34.056         -0.430         8.074           2241         CA         MET         1719         34.350         -0.490         9.501           2243         CG         MET         1719         32.408         1.060         10.194           2244         SD         MET         1719         31.015         1.307         11.314           2245         CE         MET         1719         34.998         -1.810         9.854           2246         C         MET         1719         34.998         -1.810         9.854           2247         O         MET         1719         34.998         -1.810         9.854           2248         N         ASP         1720         35.778         -1.809         10.926           2251         CA         ASP         1720         37.593         -2.630         11.358           2251         CB         ASP         1720         38.628	2237   C

ATO	DM 230	2 0	<b>~</b> 11.						
ATO			CY			~	15.49	3 1.0	0 44.63
ATC			THI		31.62		15.143		
ATO		_	THE		32.25		14.320		
ATO			THE		31.33				
ATO					30.109		13.523		
ATO			_		31.070	-16.019	15.454		• • •
ATO		_	THE		32.668		12.963		
ATO			THR		32.158	-12.593	12.518		
			ASN		33.619		12.319		
ATO			ASN		34.030		10.983	-	<del>-</del>
ATO		_	ASN		35.166		10.422		
ATO			ASN	_	36.463		11.168		
ATO				1727	37.047		11.158		
ATON			ASN	1727	36.931	-15.592	11.814	1.00	
ATON		_	ASN	1727	32.824		10.058	1.00	
ATOM			ASN	1727	32.681			1.00	34.27
MOTA			GLU	1728	31.969		9.116	1.00	32.96
ATOM			GLU	1728	30.778	-15.235	10.326	1.00	32.49
ATOM		CB	GLU	1728	30.064	-16.504	9.510	1.00	31.99
ATOM	2327	CG	GLU	1728	28.836	-16.866	9.975	1.00	34.15
ATOM	2328	CD	GLU	1728	28.187		9.156	1.00	35.63
ATOM		OE1	GLU	1728	28.200	-18.169	9.608	1.00	39.72
ATOM	2330	OE2	GLU	1728	27.654	-18.463	10.824	1.00	42.25
MOTA	2331	С	GLU	1728	29.814	-18.896	8.742	1.00	39.87
MOTA	2332	0	GLU	1728	29.309	-14.049	9.549	1.00	30.76
MOTA	2333	N	LEU	1729	29.559	-13.602	8.512	1.00	29.58
ATOM	2335	CA	LEU	1729	28.670	-13.544	10.750	1.00	30.01
ATOM	2336	CB	LEU	1729		-12.408	10.911	1.00	30.21
ATOM	2337	CG	LEU	1729	28.225	-12.272	12.364	1.00	30.13
ATOM	2338	CD1	LEU	1729	27.208	-13.350	12.748	1.00	33.61
ATOM	2339	CD2	LEU	1729	27.119	-13.483	14.262	1.00	33.71
ATOM	2340	С	LEU	1729	25.844	-13.021	12.139	1.00	30.31
ATOM	2341	0	LEU	1729	29.316	-11.133	10.390	1.00	30.26
ATOM	2342	N	TYR	1730	28.619	-10.229	9.938	1.00	28.89
ATOM	2344	CA	TYR		30.648	-11.063	10.435	1.00	28.91
ATOM	2345	CB	TYR	1730	31.343	-9.893	9.912	1.00	28.91
ATOM	2346	CG	TYR	1730	32.804	-9.861	10.359	1.00	29.09
ATOM	2347	CD1		1730	33.537	-8.639	9.857	1.00	30.15
ATOM	2348	CE1	TYR	1730	33.037	-7.358	10.103	1.00	29.97
ATOM	2349	CD2	TYR	1730	33.688	-6.227	9.626	1.00	28.99
ATOM	2350	CE2	TYR	1730	34.716	-8.757	9.119	1.00	29.24
ATOM	2351	CZ	TYR	1730	35.386	-7.620	8.632	1.00	28.25
ATOM	2352		TYR	1730	34.861	-6.362	8.889	1.00	28.41
ATOM	2354	ОН	TYR	1730	35.485	-5.227	8.405	1.00	31.64
ATOM		C	TYR	1730	31.260	-9.943	8.379	1.00	27.10
ATOM	2355	0	TYR	1730	31.078	-8.920	7.726	1.00	27.46
ATOM	2356	N	MET	1731	31.390	-11.138	7.813		26.68
ATOM	2358	CA	MET	1731	31.298	-11.315	6.372		28.68
	2359	CB	MET	1731	31.526	-12.778			
ATOM	2360	CG	MET	1731	31.158	-13.087			35.43
ATOM	2361	SD		1731	31.441	-14.804			46.19
ATOM	2362	CE	MET	1731	32.603	-14.550			60.10
ATOM	2363	С	MET	1731	29.917	-10.858			58.31
ATOM	2364	0		1731	29.782	-10.227		_	27.42
ATOM	2365	N		1732	28.893	-11.191			30.80
							6.688	1.00	28.53

ATO	DM 2367	CA	MET	1732	27.522	-10.777	6.389	1.00	26.47	
ATC	OM 2368	CB	MET	1732	26.562	-11.308	7.458	1.00	25.79	
ATC	M 2369	CG	MET	1732	25.116	-10.838	7.274	1.00	26.01	
ATC	M 2370	SD	MET	1732	24.004	-11.550	8.469	1.00	26.22	
ATC	M 2371	CE	MET	1732	23.787	-13.195	7.783	1.00	23.74	
ATO	M 2372	C	MET	1732	27.445	-9.243	6.319	1.00	25.15	
ATO	M 2373	0	MET	1732	26.886	-8.691	5.379	1.00	25.41	
ATO	M 2374	N	MET	1733	28.024	-8.564	7.308	1.00	26.48	
ATO	M 2376	CA	MET	1733	28.057	-7.104	7.331	1.00	27.09	
ATO	M 2377	CB	MET	1733	28.903	-6.594	8.488	1.00	25.91	
ATO	M 2378	CG	MET	1733	28.235	-6.556	9.824	1.00	31.64	
ATO	M 2379	SD	MET	1733	29.442	-6.111	11.094	1.00	29.59	
ATO	M 2380	CE	MET	1733	28.886	-7.126	12.420	1.00	28.14	
ATO	M 2381	C	MET	1733	28.720	-6.613	6.056	1.00	28.43	
ATO	M 2382	0	MET	1733	28.185	-5.753	5.372	1.00	31.37	
ATO	M 2383	N	ARG	1734	29.891	-7.169	5.747	1.00	28.57	
ATO	M 2385	CA	ARG	1734	30.642	-6.783	4.551	1.00	27.00	
ATO	M 2386	CB	ARG	1734	32.007	-7.488	4.510	1.00	25.98	
ATO	M 2387	CG	ARG	1734	32.927	-7.154	5.707	1.00	28.13	
ATO	M 2388	CD	ARG	1734	33.229	-5.672	5.765	1.00	29.97	
ATO	M 2389	NE	ARG	1734	33.922	-5.256	4.553	1.00	40.49	
ATO	M 2391	CZ	ARG	1734	35.238	-5.361	4.363	1.00	43.95	
ATO	M 2392	NH1	ARG	1734	36.023	-5.853	5.318	1.00	41.81	
ATO	M 2395	NH2	ARG	1734	35.760	-5.048	3.184	1.00	46.20	
ATO	M 2398	C	ARG	1734	29.859	-7.037	3.268	1.00	24.57	
ATO	M 2399	0	ARG	1734	29.992	-6.290	2.314	1.00	24.94	
ATO	M 2400	N	ASP	1735	29.071	-8.107	3.235	1.00	24.79	
ATO	M 2402	CA	ASP	1735	28.254	-8.420	2.061	1.00	23.88	
IOTA	M 2403	CB	ASP	1735	27.669	-9.830	2.150	1.00	25.95	
ATO	M 2404	CG	ASP	1735	28.724	-10.913	2.024	1.00	27.60	
ATO	M 2405	OD1	ASP	1735	29.842	-10.632	1.529	1.00	27.75	
ATO		OD2	ASP	1735	28.432	-12.051	2.430	1.00	28.90	
ATO		С	ASP	1735	27.139	-7.396	1.941	1.00	22.61	
ATO		0	ASP	1735	26.777	-6.996	0.833	1.00	22.66	
OTA		N	CYS	1736	26.611	-6.965	3.085	1.00	20.61	
ATO		CA	CYS	1736	25.561	-5.952	3.109	1.00	23.63	
ATO		CB	CYS	1736	25.007	-5.767	4.534	1.00	21.98	
ATO		SG	CYS	1736	23.934	-7.126	5.111	1.00	22.95	
ATO		С	CYS	1736	26.129	-4.633	2.599	1.00	23.62	
ATO		0	CYS	1736	25.403	-3.797	2.047	1.00	22.15	
ATO		N	TRP	1737	27.438	-4.461	2.775	1.00	24.37	
ATO		CA	TRP	1737	28.123	-3.247	2.342	1.00	23.77	
ATO		CB	TRP	1737	29.162	-2.810	3.371	1.00	19.38	
ATON		CG	TRP	1737	28.601	-2.520	4.718	1.00	21.62	
ATON		CD2	TRP	1737	29.268	-2.688	5.971	1.00	24.81	
ATON		CE2	TRP	1737	28.371	-2.278	6.980	1.00	25.95	
ATON		CE3	TRP	1737	30.534	-3.165	6.340	1.00	29.02	
ATOM		CD1	TRP	1737	27.359	-2.024	5.007	1.00	23.21	
ATON		NE1	TRP	1737	27.213	-1.876	6.362	1.00	21.80	
ATON		CZ2	TRP	1737	28.710	-2.305	8.347	1.00	26.68	
ATON		CZ3	TRP	1737	30.873	-3.198	7.699	1.00	31.06	
ATON		CH2	TRP	1737	29.959	-2.774	8.685	1.00	30.18	
ATON		C	TRP	1737	28.788	-3.372	0.978	1.00	24.88	
ATOM	1 2431	0	TRP	1737	29.737	-2.646	0.689	1.00	25.11	

	3.50						-01				
	ATOM	2432	N	HIS	1738	20 -					
	ATOM	2434	CA	HIS		28.3		. 278	0.132	1.00	0.5
	ATOM	2435	CB	HIS	1738	28.8	88 -4	.406	1.191		25.27
	ATOM	2436	CG		1738	28.2	30 -5		1.986	1.00	24.27
	<b>.</b>	2437	CD2	HIS	1738	29.1				1.00	25.24
	3 mass	2438		HIS	1738	29.72			3.081	1.00	26.28
			ND1	HIS	1738	29.69			4.147	1.00	25.67
		2440	CEl	HIS	1738	30.52	_		3.098	1.00	27.55
		2441	NE2		1738			478 -	4.117	1.00	27.51
		443	C		1738	30.56		329 -	4.770	1.00	
A	TOM 2	444	_			28.71	5 -3.		1.953	1.00	30.93
A	TOM 2	445	. = '		1738	27.65	9 -2.		1.905		25.59
A			'		1739	29.78	4 -2.			1.00	22.01
					1739	29.75	-1.4		2.612	1.00	23.84
	_			ALA j	1739	31.131			.388	1.00	24.93
			C 2		739	28.671			.024	1.00	26.39
			) ]		739	27.063			.462	1.00	25.35
	rom 24	151 h	1 V		740	27.963	-0.5		.727	1.00	
	TOM 24	53 (				28.543	-2.6		.073	1.00	28.20
Ρ	OM 24	_	•	_	740	27.528	-2.9				22.68
AT					740	27.995	-3.9			1.00	26.46
AT			•		740	27.063	-4.0		.117	1.00	29.70
AT			G2 V	AL 1	740	29.433	2.0		. 334		26.01
AT		_	V		740	26.213	-3.6		537		31.22
		_	V		740	20.213	-3.3				25.07
AT		59 N	PF		741	26.138	-4.47	74 -4.	_		
ATO		o CI			41	25.155	-2.5]	19 -5.			23.55
ATO	DM 246	51 C/				25.133	-1.19	0 -6.			25.30
ATC	DM 246				41	23.844	-2.83			.00 2	22.43
ATC	M 246					22.962	-1.67	,		.00 2	4.09
ATO					41	23.928				.00 2	3.12
ATO	• •	_	PR	0 17	41	23.272	-0.52	-		.00 2	2.04
		-	PR			22.727	-4.19				2.18
ATO			SE			22.727	-4.90			_	1.23
ATO		B CA				23.437	-4.57	0 -6.5			
ATO		9 CB	SE			22.928	-5.84	7 -7.0			3.87
ATO	M 247(					23.071	-5.907				4.36
ATON		-	SEF		_	24.436	-6.025		• •		7.39
ATOM	1 2473	_	SER		2 2	23.636	-7.058			00 29	9.25
ATOM		_	SER	174	2 2	3.145					. 96
ATOM			GLN	174	3 2	4.810	-8.179				.30
			GLN			5.550	-6.839	-5.9	15 1.		.39
ATOM			GLN	174		5.558	-7.934	-5.34	15 1.		.15
ATOM		CG	GLN			7.046	-7.755	~5.63			. 15
ATOM	2479	CD	GLN			7.359	-7.784	-7.12	6 7		. 83
ATOM	2480	OE1		1743		6.816	-9.036	-7.80	_		. 84
ATOM	2481	NE2	GLN	1743	_	7.318	-10.135	-7.59			. 20
ATOM	2484		GLN	1743	25	5.775	-8.871	-7.59			. 50
ATOM		C	GLN	1743	25	5.309	0.871	-8.62	8 1.0	0 22.	45
	2485	0	GLN	1743		816	-8.171	-3.86	8 1.0	0 23.	
ATOM	2486	N	ARG	1744		,.010	-9.135	~3.31	7 1.0	0 24.	
ATOM	2488	CA	ARG	1744		.557	-7.280	-3.22	5 1.0	•	
ATOM	2489	CB	ARG			.242	-7.424	-1.80	_		67
ATOM	2490	CG		1744	23	.699	-6.110	-1.23			
ATOM	2491		ARG	1744	24		-4.959	1 22			
ATOM		CD	ARG	1744	24			-1.338		21.	
ATOM	2492	NE	ARG	1744	24		-3.640	-0.890		20.	
	2494	CZ	ARG	1744			-2.552	-1.305	1.00		
ATOM	2495	NH1	ARG	1744		.540	-1.313	-1.583	1.00		
ATOM	2498	NH2	ARG		23,	. 257 .	0.955	-1.481			
ATOM	2501	C		1744	25.	450 -	0.448	-2.036		_	14
		_	ARG	1744	23.		8.505	-1.640			
SSSD/55	14501							4.040	1.00	22.5	3



MOTA	2502	0	ARG	1744	22.437	-8.800	-2.588	1.00	23.08
ATOM	2503	N	PRO	1745	23.162	-9.170	-0.467	1.00	20.76
MOTA	2504	CD	PRO	1745	24.087	-9.078	0.681	1.00	21.71
ATOM	2505	CA	PRO	1745	22.160	-10.207	-0.243	1.00	22.34
ATOM	2506	CB	PRO	1745	22.632	-10.859	1.057	1.00	20.58
MOTA	2507	CG	PRO	1745	23.298	-9.727	1.783	1.00	20.36
MOTA	2508	C	PRO	1745	20.814	-9.512	-0.048	1.00	23.62
MOTA	2509	0	PRO	1745	20.759	-8.318	0.255	1.00	25.29
ATOM	2510	N	THR	1746	19.731	-10.235	~0.275	1.00	23.39
ATOM	2512	CA	THR	1746	18.404	-9.675	-0.080	1.00	22.77
ATOM	2513	CB	THR	1746	17.386	-10.368	-1.004	1.00	23.24
MOTA	2514	OG1	THR	1746	17.409	-11.783	-0.763	1.00	23.11
MOTA	2516	CG2	THR	1746	17.724	-10.103	-2.475	1.00	24.96
ATOM	2517	C	THR	1746	18.009	-9.954	1.365	1.00	24.98
ATOM	2518	0	THR	1746	18.664	-10.758	2.043	1.00	24.30
MOTA	2519	N	PHE	1747	16.944	-9.318	1.853	1.00	24.95
ATOM	2521	CA	PHE	1747	16.501	-9.596	3.221	1.00	25.16
MOTA	2522	CB	PHE	1747	15.395	-8.628	3,661	1.00	23.64
MOTA	2523	CG	PHE	1747	15.916	-7.283	4.089	1.00	24.34
ATOM	2524	CD1	PHE	1747	16.715	-7.167	5.226	1.00	21.21
MOTA	2525	CD2	PHE	1747	15.649	-6.137	3.334	1.00	21.42
ATOM	2526	CE1	PHE	1747	17.252	-5.932	5.597	1.00	20.99
ATOM	2527	CE2	PHE	1747	16.178	-4.907	3.699	1.00	20.36
ATOM	2528	CZ	PHE	1747	16.985	-4.807	4.840	1.00	19.30
ATOM	2529	C	PHE	1747	16.034	-11.049	3.311	1.00	23.57
ATOM	2530	O	PHE	1747	16.182	-11.702	4.344	1.00	25.32
ATOM	2531	N	LYS	1748	15.520	-11.573	2.202	1.00	23.19
ATOM	2533	CA	LYS	1748	15.066	-12.958	2.167	1.00	23.67
ATOM	2534	СВ	LYS	1748	14.462	-13.285	0.799	1.00	26.67
ATOM	2535	CG	LYS	1748	14.018	-14.739	0.622	1.00	30.49
ATOM	2536	CD	LYS	1748	13.642	-14.996	-0.837	1.00	38.98
ATOM	2537	CE	LYS	1748	13.182	-16.432	-1.087	1.00	44.52
MOTA	2538	NZ	LYS	1748	11.997	-16.790	-0.245	1.00	52.75
ATOM	2542	С	LYS	1748	16.264	-13.865	2.445	1.00	25.65
ATOM	2543	0	LYS	1748	16.184	-14.778	3.270	1.00	27.19
MOTA	2544	N	GLN	1749	17.378	-13.603	1.762	1.00	24.56
MOTA	2546	CA	GLN	1749	18.588	-14.397	1.950	1.00	26.33
MOTA	2547	CB	GLN	1749	19.702	-13.953	0.993	1.00	27.97
MOTA	2548	CG	GLN	1749	19.416	-14.066	-0.484	1.00	37.31
MOTA	2549	CD	GLN	1749	20.518	-13.415	-1.315	1.00	40.24
MOTA	2550	OE1	GLN	1749	20.296	-12.408	-1.970	1.00	38.83
ATOM	2551	NE2	GLN	1749	21.726	-13.983	-1.259	1.00	47.83
ATOM	2554	С	GLN	1749	19.099	-14.223	3.377	1.00	23.92
ATOM	2555	0	GLN	1749	19.459	-15.196	4.040	1.00	25.27
ATOM	2556	N	LEU	1750	19.155	-12.976	3.829	1.00	23.12
MOTA	2558	CA	LEU	1750	19.641	-12.662	5.175	1.00	24.34
MOTA	2559	CB	LEU	1750	19.607	-11.149	5.427	1.00	23.08
MOTA	2560	CG	LEU	1750	20.633	-10.311	4.665	1.00	23.84
ATOM	2561	CD1	LEU	1750	20.274	-8.806	4.724	1.00	22.10
ATOM	2562	CD2	LEU	1750	22.013	-10.586	5.246	1.00	24.91
ATOM	2563	С	LEU	1750	18.840	-13.400	6.236	1.00	27.40
ATOM	2564	0	LEU	1750	19.408	-13.915	7.211	1.00	27.11
ATOM	2565	N	VAL	1751	17.527	-13.482	6.031	1.00	26.83
ATOM	2567	CA	VAL	1751	16.665	-14.174	6.970	1.00	25.31
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						1;	96			
A'	TOM 2	568	CB v	/AL 175						
A:					-0.2		-13.9		599 1.	00 25.87
A							-14.9		_	00 28.43
ΑT			_		• •		-12.5	93 6.9		00 21.52
AT	OM 25						-15.6			00 25.87
AT		573 N	_ *				~16.2	18 8.1		-5.0,
AT		_					-16.2			
AT							-17.6	51 5.7		
AT							-18.1	34 4.3		
AT			_		2,		-18.0	77 3.6		
AT	_				-0.5		-18.5	75 2.2		
ATO							-18.12			
ATO	OM 25		-				-19.42		02 1.0	
ATC	DM 25						-17.89	6.46		
ATC	DM 258		AS				-18.84	7 7.23		
ATC	M 258						17.01	1 6.18		
ATC	M 258				,		17.13	1 6.77		
ATO	M 258						16.10			
ATO	M 258				22.48		16.34	4 4.67		
ATO					22.36		17.49			
ATO			AS:		22.81		15.37	3.95		38.26
ATO		_	ASI	_	21.21		16.968	8.28		
ATO	M 259		LE		21.739		17.800	9.02		
ATO	M 259			_	20.53		15.926		3 1.00	
ATON	1 259		LEU		20.421		15.673			
ATON	,		LEU		19.754		14.328		1.00	
ATOM					20.733		13.199		1.00	24.47
ATOM					20.007		1.863			
ATOM	2599		LEU		21.846		.3.207		1.00	
ATOM	2600	0	LEU		19.688		6.789	10.921	1.00	
MOTA		N	ASP		20.037		7.135	12.048	1.00	32.64
ATOM		CA	ASP	1755	18.690		7.367	10.259		32.61
ATOM		CB	ASP	1755	17.931		8.460	10.833	1.00	34.20
ATOM	2605	CG	ASP	1755	16.823 15.808		8.883	9.872	1.00	37.70
ATOM	2606		ASP	1755			9.780	10.526	1.00	44.27
ATOM	2607	OD2	ASP	1755	15.445		9.521	11.692	1.00	47.16
ATOM	2608	C	ASP	1755	15.370 18.894	-2	0.745	9.876	1.00	51.35
MOTA	2609	0	ASP	1755	18.858	-19	9.616	11.073	1.00	34.63
ATOM	2610	N	ARG	1756	19.782		2.273	12.119	1.00	36.24
ATOM	2612	CA	ARG	1756	20.784		9.826	10.108	1.00	32.60
ATOM	2613	CB	ARG	1756	21.548		870	10.190	1.00	33.69
ATOM	2614	CG	ARG	1756	22.639		939	8.867	1.00	35.42
ATOM	2615	CD	ARG	1756	23.212		.003	8.800	1.00	40.87
MOTA	2616	NE	ARG	1756	23.739	-22	.094	7.395	1.00	42.73
ATOM	2618	CZ	ARG	1756	24.882		.813	6.926	1.00	48.45
ATOM	2619	NH1	ARG	1756	25.634		.274	7.340	1.00	49.90
ATOM	2622.	NH2	ARG	1756	25.276	-20	. 905	8.243	1.00	49.63
ATOM	2625	C	ARG	1756	21.748	-19	.105	6.844	1.00	50.86
ATOM	2626	0	ARG	1756	21.929		.598	11.345	1.00	34.78
ATOM	2627	N	ILE	1757	22.325	-21	.436	12.228	1.00	36.24
ATOM	2629	CA	ILE	1757	23.281	-19	.402	11.363	1.00	35.35
ATOM	2630	CB	ILE	1757	23.281	-19	.018	12.392	1.00	35.54
ATOM	2631	CG2	ILE	1757	24.955	-17	.631	12.103	1.00	34.99
ATOM	2632	CG1	ILE	1757	24.955	~17.	303	13.159	1.00	32.06
SSCD/FF					/	-17.	626	10.711	1.00	33.77
SELECT ACE										





							-					
							-16.2	47 1	0.185	1.00	31.	.44
MOTA	2633	CD1	ILE	1757			-19.0		3.803	1.00	36.	
MOTA	2634	C	ILE	1757		22.698	-19.5		4.716	1.00		. 40
MOTA	2635	0	ILE	1757		23.337	-18.5		13.988	1.00		.91
MOTA	2636	N	VAL	1758		21.487	-18.4		15.322	1.00		. 68
ATOM	2638	CA	VAL	1758		20.881	-17.5		15.312	1.00		.77
ATOM	2639	CB	VAL	1758		19.425	-18.		16.708	1.00	38	.39
ATOM	2640	CG1	VAL	1758		18.806	-16.		14.854	1.00		.69
ATOM	2641	CG2	VAL	1758		19.392	-19.		15.895	1.00		.38
MOTA	2642	С	VAL	1758		20.891	-20.	_	16.997	1.00		.41
MOTA	2643	0	VAL	1758		21.405 20.379	-20.		15.111	1.00		.59
MOTA	2644	N	ALA	1759		20.375	-22.	_	15.508	1.00		.84
MOTA	2646	CA	ALA	1759		19.741	-23.		14.384	1.0	-	.20
MOTA	2647	CB	ALA	1759			-22.		15.897	1.0		2.52
ATOM	2648	С	ALA	1759		21.703	-23.		16.809	1.0		1.78
ATOM	2649	0	ALA	1759		21.822		339	15.208	1.0		3.16
ATOM	2650	N	LEU	1760		22.740		.800	15.493	1.0		6.98
MOTA	2652	CA	LEU			24.095	-22	.761	14.203	1.0		7.66
MOTA	2653	CB	LEU			24.921		.545	13.060	1.0		2.77
MOTA	2654	CG	LEU			24.286		.222	11.745	1.0		6.58
ATOM	2655	CD1				24.973	-25	.038	13.369	1.0		3.06
MOTA	2656	CD2				24.343	-21	.986	16.573	1.0		7.43
ATOM		C	LEU			24.811 25.917		.335	16.989	1.0		6.58
ATOM		3 0	LEU			24.183		.914	17.034	1.0		8.65
ATOM		N	THE			24.103		.055	18.021	1.		19.69
ATOM		L CA	THE			24.814		3.570	17.831	1.		50.15
ATOM		2 CB	TH			24.382		3.127	16.529			49.87
ATON						25.063		7.671	18.843	1.		48.64
MOTA						24.673		0.497	19.475			50.33
OTA			TH			23.584		0.825	19.947			48.81
ATO	M 266	7 0	TH			25.811		0.511	20.166			50.25
ATO	м 266		SE	_		25.891		0.890	21.56			50.98
OTA						27.362		0.887	22.00			54.71
ATO	M 267				62	27.53		1.423	23.30		.00	57.99 49.39
OTA	M 267			_	62 62	25.08		9.914	22.42		.00	49.39
ATO			SI		62	25.29		8.694	22.37		.00	48.84
ATC						79.62		5.766	14.53		.00	46.93
OTA				_	51	79.56	6 2	24.645			.00	46.66
OTA					51	78.27	6 2	23.838		_	.00	43.02
TA		_	_		61	79.67		25.114	12.13		.00	40.19
TA		78 C	_		61	79.69	2 :	24.301			.00	41.48
TA		79 0	_		62	79.79		26.42	7 11.95		00	39.59
TA	_	80 N			62	79.90		27.034	10.62	-	00	40.66
TA					62	80.02		28.56	0 10.74		1.00	36.60
ΤA					62	81.0		26.48	0 9.7		1.00	35.10
AT	-	184 C	_		62	80.8		26.12	1 8.6		1.00	36.07
PA		185 C	_		63	82.2		26.41	6 10.3		1.00	35.60
PΑ		-	_	_	163	83.4		25.91	6 9.6		1.00	
A'l	_					84.5		26.90	6 9.7	-	1.00	38.15
A7				_	163	84.3		28.10	4 8.8	-	1.00	44.08
A.				_	463	84.1		29.36	8 9.4		1.00	44.99
A'	rom 3				463	83.8		30.45	51 8.5		1.00	46.88
A'					463 463			27.99	59 7.4		1.00	43.95
					463 463			29.04		642	1.00	41.86
A	TOM 3	494	CE2	TYR	-203							



							1.0	.0				
	ATOM	3495	CZ	TYR	463	_						
	ATOM	3496	ОН	TYR	463	,		30.	282 7	.215	1.00	42
i	ATOM	3498	С	TYR	463		68	31.	364 6	.431	1.00	
7	MOTA	3499	0	TYR	463		03	24.5		.014	1.00	
7	MOT!	3500	N	GLU	463	84.4	40	23.8		.147	1.00	33.90
7	MOTA	3502	CA	GLU	464	83.7	42	24.0		.260	1.00	33.90
A	TOM 3	3503	CB	GLU	464	84.1	67	22.7		. 633	1.00	32.81
	TOM 3	504	CG	GLU	464	85.66		22.7		. 919		34.64
A				GLU	464	86.07		23.6		049	1.00	37.48
A					464	87.55		23.9		015	1.00	45.48
A'				GLU.	464	87.92	0	24.9		659	1.00	55.80
· A:			_	GLU	464	88.34	4	23.2		351	1.00	61.78
A7			_	GLU	464	83.42	6	22.29		858	1.00	58.34
				GLU	464	83.08		23.11			1.00	33.05
				EU	465	83.14		21.00			1.00	34.54
				EU	465	82.462		20.46			1.00	32.59
					465	81.484		19.34			1.00	33.74
AT	_				465	80.510		19.43			1.00	31.20
AT				EU	465	79.355					1.00	32.77
AT				EU .	465	80.021		18.49	_ '		1.00	26.22
ATO			~	EU .	465	83.511		0.84			1.00	31.59
ATO				EU 4	465	84.641		9.889	-		1.00	35.64
ATO			P	RO 4	166	83.150		9.574	_		1.00	33. <b>7</b> 7
ATO			D bi	RO 4	166	81.865		9.734				36.71
ATO			A bi		66	84.074	2	0.104			1.00	36.97
			3 PF		66	83.247	1	9.185				36.17
ATO			PR	0 4	66	82.274	1	9.196				36.83
ATO		_	PR	_	66	84.419	20	326		94 1		10.80
ATO		-	PR		66		17	7.765		50 <u>1</u>		7.39
ATO	_		GL		67	83.626		7.077	16.29			4.71
ATO			GL		57	85.611		.330	17.31			8.40
ATON			GL		57	86.030		. 987	16.97	-		2.59
ATON			GL	J 46		87.493		.987	16.54		-	9.21
ATOM			GL			87.922		.682	15.89			B.93
ATOM	-004	OE:				89.276		. 769	15.21			4.76
ATOM		OE2				90.013		.767	15.42	_		3.57
ATOM		C	GLU			89.592		. 823	14.458			9.03
ATOM		0	GLU			85.825		.037	18.146		_	
ATOM			ASP			85.938	15.	430	19.309			74
ATOM	3538	CA	ASP	46		85.472	13.	802	17.831			52
ATOM	3539	CB	ASP			85.273	12.	776	18.851			.57
ATOM	3540	CG	ASP	468		83.793	12.	640	19.224			. 86
ATOM	3541	OD1	ASP	468		83.566	11.	697	20.397			.27
ATOM	3542	OD2	ASP	468		82.429	11.	670	20.919	1.0		. 36
ATOM	3543	C		468		84.514	10.		20.807			.50
ATOM	3544	o	ASP	468		85.803	11.		18.278	1.0		. 55
ATOM	3545	N	ASP	468		85.068	10.		17.650	1.0		
ATOM	3546		PRO	469	-	87.100	11.2			1.0		.80
ATOM	3547	CD	PRO	469	8	38.001	12.0		18.481	1.0	•	
ATOM	3548	CA	PRO	469	ε	37.801	10.0		19.276	1.0		
ATOM		CB	PRO	469	8	9.091	10.0		18.012	1.0		
ATOM	3549	CG	PRO	469	8	9.366	11.5		18.831	1.0	0 40.	
ATOM	3550	C	PRO	469	8	7.033			18.938	1.00	0 39.	
ATOM	3551	0	PRO	469	8	7.032	8.7		18.260	1.00		
ATOM	3552	N	ARG	470		6.361	7.8		17.414	1.00		
MULA	3554	CA	ARG	470		5.600	8.6		19.411	1.00		
CCCD :=-					•	000	7.4	46 ]	9.779	1.00		
SSSD/55	145 001											-





ATOM	3555	CB	ARG	470	84.827	7.677	21.075	1.00	44.18
ATOM	3556	CG	ARG	470	85.628	8.240	22.218	1.00	47.89
MOTA	3557	CD	ARG	470	84.719	8.518	23.400	1.00	50.56
MOTA	3558	NE	ARG	470	83.576	9.345	23.023	1.00	51.20
MOTA	3560	CZ	ARG	470	82.695	9.845	23.881	1.00	52.24
ATOM	3561	NH1	ARG	470	82.818	9.608	25.183	1.00	51.31
ATOM	3564	NH2	ARG	470	81.672	10.564	23.432	1.00	52.73
ATOM	3567	С	ARG	470	84.596	7.004	18.723	1.00	39.03
ATOM	3568	0	ARG	470	84.401	5.813	18.518	1.00	40.72
ATOM	3569	N	TRP	471	83.972	7.965	18.050	1.00	37.77
ATOM	3571	CA	TRP	471	82.948	7.656	17.059	1.00	36.73
MOTA	3572	CB	TRP	471	81.672	8.401	17.432	1.00	35.05
ATOM	3573	CG	TRP	471	81.044	7.862	18.673	1.00	34.85
ATOM	3574	CD2	TRP	471	80.235	6.687	18.766	1.00	34.96
ATOM	3575	CE2	TRP	471	79.831	6.564	20.116	1.00	35.12
MOTA	3576	CE3	TRP	471	79.810	5.721	17.838	1.00	33.25
ATOM	3577	CD1	TRP	471	81.106	8.390	19.933	1.00	29.97
ATOM	3578	NE1	TRP	471	80.377	7.616	20.805	1.00	32.18
ATOM	3580	CZ2	TRP	471	79.017	5.512	20.560	1.00	33.98
ATOM	3581	CZ3	TRP	471	79.002	4.673	18.282	1.00	33.71
ATOM	3582	CH2	TRP	471	78.618	4.580	19.632	1.00	33.28
ATOM	3583	C	TRP	471	83.275	7.930	15.599	1.00	37.27
ATOM	3584	0	TRP	471	82.580	7.445	14.695	1.00	36.61
ATOM	3585	N	GLU	472	84.341	8.680	15.361	1.00	37.93
ATOM	3587	CA	GLU	472	84.706	9.054	14.004	1.00	37.08
ATOM	3588	CB	GLU	472	85.865	10.049	14.045	1.00	36.30
ATOM	3589	CG	GLU	472	86.026	10.851	12.773	1.00	33.51
MOTA	3590	CD	GLU	472	84.931	11.895	12.580	1.00	33.80
ATOM	3591	OE1	GLU	472	84.385	12.408	13.581	1.00	35.19
MOTA	3592	OE2	GLU	472	84.641	12.226	11.412	1.00	32.51
MOTA	3593	С	GLU	472	85.021	7.923	13.032	1.00	37.88
ATOM	3594	0	GLU	472	85.774	7.000	13.351	1.00	38.20
ATOM	3595	N	LEU	473	84.422	7.992	11.846	1.00	37.55
ATOM	3597	CA	LEU	473	84.678	7.004	10.813	1.00	36.93
ATOM	3598	CB	LEU	473	83.404	6.244	10.443	1.00	37.08
ATOM	3599	CG	LEU	473	83.680	5.086	9.470	1.00	39.14
MOTA	3600	CD1	LEU	473	84.196	3.877	10.250	1.00	38.39
MOTA	3601	CD2	LEU	473	82.433	4.716	8.672	1.00	39.46
MOTA	3602	С	LEU	473	85.207	7.732	9.577	1.00	38.52
MOTA	3603	0	LEU	473	84.660	8.764	9.182	1.00	38.67
ATOM	3604	N	PRO	474	86.334	7.259	9.005	1.00	39.02
MOTA	3605	CD	PRO	474	87.259	6.259	9.571	1.00	38.39
ATOM	3606	CA	PRO	474	86.918	7.877	7.809	1.00	38.24
ATOM	3607	CB	PRO	474	88.188	7.049	7.590	1.00	38.40
ATOM	3608	CG	PRO	474	88.580	6.680	8.979	1.00	35.50
ATOM	3609	C	PRO	474	85.942	7.727	6.642	1.00	37.56
MOTA	3610	0	PRO	474	85.415	6.641	6.400	1.00	37.88
MOTA	3611	N	ARG	475	85.720	8.809	5.907	1.00	37.73
ATOM	3613	CA	ARG	475	84.779	8.790	4.795	1.00	40.01
MOTA	3614	CB	ARG	475	84.655	10.183	4.182	1.00	38.31
MOTA	3615	CG	ARG	475	84.217	11.236	5.198	1.00	35.15
MOTA	3616	CD	ARG	475	84.069	12.631	4.586		33.92
ATOM	3617	NE	ARG	475	83.718	13.603	5.616	1.00	30.45
MOTA	3619	CZ	ARG	475	82.475	13.880	5.993	1.00	26.48

	TOM :	3620	NH1	ARG	475	81 44						
		3623	NH2		475	81.44		284	5.4	07 1	.00	24.80
		626			475	82.27		650	7.0		.00	25.16
		627	_		175	85.05	-	735	3.7		.00	42.18
		628		_	176	84.12	-	197	3.1		.00	41.43
		630			176	86.32	-	391	3.5		.00	45.44
		631		_	76	86.67		387	2.54		.00	49.80
AT	COM 3	632			76	88.19		343	2.32		. 00	50.95
ΓA	OM 3				76	88.944		975	3.58	· ·	00	53.89
AT	'OM 36	534 (			76	89.303	· =	789	3.73		00	59.71
AT	'OM 36	535 (		_	76	89.176		367	4.42		00	57.39
AT	OM 36	36 (			76	86.149	_		2.95		00	51.23
AT	OM 36	37 N			70 77	86.051			2.12		00	53.54
ATO	OM 36	39 0			, , 77	85.814			4.23			50.49
ATO						85.285	3.6	10	4.75			
ATO	DM 36					85.834	3.3	64	6.152			49.32
ATC	OM 36					87.237	2.8		6.112			49.79
ATC	DM 36			_		87.960	2.9	81	7.420			53.06
ATC						87.310	2.2		8.529			56.76
ATO		-		- •		87.728	2.3		9.789			59.35
ATO						88.793	3.10		10.101			62.23
ATO.	M 365		12 Ar Ar			87.067	1.74		10.745		_	63.66
ATO		_		- •		83.755	3.54		4.750			64.35
ATO			AR			83.160	2.69		5.404			18.04
ATO			LE			83.129	4.41		3.958	-		18.09
ATON	_					81.685	4.46		3.870	1.0		15.38
ATOM						81.168	5.57		4.790	1.0		1.60
ATOM						79.651	5.69		4.894	1.0		8.39
ATOM				•		79.113	4.59		5.802	1.00		6.38
ATOM						79.293	7.06		5.441	1.00		3.98
ATOM			LEC			81.279	4.774		2.433	1.00		0.06
ATOM		_	LEU			81.696	5.780	_	1.870	1.00		1.92
ATOM			VAL	•		80.466	3.904		1.844	1.00		3.99
ATOM			VAL			79.992	4.082			1.00		2.29
ATOM			VAL			80.227	2.816		0.471	1.00		L.07
ATOM	3668	_				79.719	3.057		0.397	1.00		1.13
ATOM				479		81.700	2.448		.810	1.00		19
ATOM	3669 3670	•	VAL	479		78.500	4.345		.420	1.00		.36
ATOM	3671	_	VAL	479		77.719	3.451		.540	1.00		.44
ATOM	3673	N	LEU	480		78.112	5.582		.885	1.00		.86
ATOM		CA	LEU	480		76.706	5.973		.253	1.00		.37
ATOM	3674	CB	LEU	480		76.568	7.492		.293	1.00		.63
ATOM	3675	CG	LEU	480		77.236	8.332		.166	1.00		. 91
ATOM	3676	CD1	LEU	480		76.890	9.800		.261	1.00	39	. 23
ATOM	3677	CD2	LEU	480		76.791				1.00	37	. 73
	3678	С	LEU	480		75.899	7.877			1.00	35.	18
ATOM	3679	0	LEU	480		76.395	5.273			1.00	42.	
ATOM	3680	N	GLY	481		74.650	5.048		890	1.00	45.	
ATOM	3682	CA	GLY	481		73.812	4.947		476	1.00	41.	
ATOM	3683	C	GLY	481		72.446	4.257		433	1.00	40.	
MOTA	3684	0	GLY	481	7	2.446	4.872			1.00	41.	
MOTA	3685	N	LYS	482	7	4.404	6.091		550	1.00	41.	
ATOM	3687	CA	LYS	482	,	1.474	4.009	-1.		1.00	42.	
ATOM	3688	CB	LYS	482		0.105	4.429	-2.	166 ]	1.00	44.	
ATOM	3689	С	LYS	482		9.240	3.221	-2.		.00	45.	
				102	ь	9.475	5.148	-0.		.00	44.	
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ATOM	3690	0	LYS	482	69.638	4.752	0.155	1.00	45.23
ATOM	3691	N	PRO	483	68.749	6.234	-1.273	1.00	45.94
MOTA	3692	CD	PRO	483	68.518	6.880	-2.576	1.00	46.96
ATOM	3693	CA	PRO	483	68.099	6.983	-0.206	1.00	47.79
MOTA	3694	CB	PRO	483	67.542	8.200	-0.947	1.00	47.02
MOTA	3695	CG	PRO	483	67.269	7.666	-2.307	1.00	46.65
MOTA	3696	C	PRO	483	66.991	6.151	0.429	1.00	48.74
ATOM	3697	0	PRO	483	66.314	5.376	-0.251	1.00	48.01
ATOM	3698	N	LEU	484	66.858	6.268	1.742	1.00	49.91
ATOM	3700	CA	LEU	484	65.837	5.547	2.477	1.00	53.93
MOTA	3701	CB	LEU	484	66.433	4.883	3.720	1.00	50.17
MOTA	3702	CG	LEU	484	67.517	3.844	3.445	1.00	48.93
MOTA	3703	CD1	LEU	484	68.226	3.460	4.731	1.00	49.05
ATOM	3704	CD2	LEU	484	66.906	2.630	2.784	1.00	47.03
MOTA	3705	С	LEU	484	64.715	6.501	2.878	1.00	58.70
ATOM	3706	0	LEU	484	63.571	6.075	3.055	1.00	61.95
ATOM	3707	N	GLY	485	65.027	7.788	3.006	1.00	60.35
ATOM	3709	CA	GLY	485	63.998	8.737	3.397	1.00	64.00
MOTA	3710	С	GLY	485	64.445	10.183	3.476	1.00	66.09
MOTA	3711	0	GLY	485	65.643	10.468	3.577	1.00	65.26
MOTA	3712	N	GLU	486	63.471	11.090	3.458	1.00	67.18
ATOM	3714	CA	GLU	486	63.733	12.525	3.508	1.00	68.69
ATOM	3715	CB	GLU	486	63.873	13.084	2.091	1.00	69.88
ATOM	3716	С	GLU	486	62.618	13.249	4.245	1.00	68.80
ATOM	3717	0	GLU	486	61.481	12.775	4.295	1.00	69.26
MOTA	3718	N	GLY	487	62.943	14.415	4.791	1.00	68.47
ATOM	3720	CA	GLY	487	61.960	15.188	5.520	1.00	67.56
ATOM	3721	C	GLY	487	62.373	16.635	5.634	1.00	66.71
ATOM	3722	0	GLY	487	63.040	17.172	4.747	1.00	66.48
ATOM	3723	N	ALA	488	61.979	17.265	6.735	1.00	67.22
ATOM	3725	CA	ALA	488	62.304	18.661	6.992	1.00	67.78
ATOM ATOM	3726 3727	CB	ALA	488	61.637	19.121	8.283	1.00	68.97
MOTA		C	ALA	488	63.817	18.830	7.085	1.00	67.38
ATOM	3728 3729	0	ALA	488	64.413	18.597	8.141	1.00	67.14
ATOM	3729	N CA	PHE	489	64.429	19.155	5.946	1.00	66.22
ATOM	3732	CB	PHE PHE	489	65.877	19.364	5.831	1.00	65.49
ATOM	3733	CP	PHE	489 489	66.277	20.699	6.467	1.00	66.11
ATOM	3734	0	PHE	489	66.749 67.924	18.207	6.368	1.00	64.07
ATOM	3735	N	GLY	490	66.171	18.399	6.731	1.00	61.56
MOTA	3737	CA	GLY	490	66.852	17.005 15.803	6.349 6.797	1.00	60.79
ATOM	3738	C	GLY	490	66.787	14.760		1.00	54.72
ATOM	3739	ō	GLY	490	65.765	14.760	5.692 5.013	1.00	51.78
ATOM	3740	N	GLN	491	67.874	14.015	5.528		49.17
ATOM	3742	CA	GLN	491	68.000	12.984		1.00	49.97
ATOM	3743	CB	GLN	491	68.891	13.520	4.504	1.00	48.06
ATOM	3744	CG	GLN	491	69.286		3.371	1.00	51.02
ATOM	3745	CD	GLN	491	70.155	12.518	2.289	1.00	56.00
ATOM	3746	OE1	GLN	491	70.155	13.143 14.330	1.202	1.00	58.93
ATOM	3747	NE2	GLN	491	70.529		1.255	1.00	60.31
ATOM	3750	C	GLN	491	68.623	12.341	0.202	1.00	60.19
ATOM	3751	0	GLN	491	69.511	11.720	5.114	1.00	45.59
ATOM	3752	N	VAL	492	68.148	11.792	5.959	1.00	45.22
ATOM	3754	CA	VAL	492	68.676	10.561 9.304	4.693	1.00	43.19
			4	774	00.070	J.3U4	5.193	1.00	41.54

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		3755	CB	VAL	492	67.6	5.5	0 55.				
		3756	CG1	VAL	492	68.2		8.584			1.00	41.74
		3757	CG2	VAL	492	67.2	_	7.248	6.5	661	1.00	43.70
		3758	C	VAL	492		_	9.463	7.2	69 ]	1.00	44.07
		3759	0	VAL	492	68.9		3.424	3.9		.00	39.72
		3760	N	VAL	493	68.1	25 g	3.271	3.1		.00	
A	TOM 3	762	CA	VAL		70.1		7.872	3.9		.00	39.81
A	P1011	763	CB	VAL	493	70.54	15 7	.001	2.8			36.38
A'			CG1		493	71.58	30 7	.666	1.8		.00	35.88
A.				VAL	493	71.14		.069			.00	36.92
			_	VAL	493	72.97		.670	1.4		.00	36.64
				VAL	493	71.13			2.46		.00	38.29
			0	VAL	493	71.69		.689	3.39		.00	36.03
			N :	LEU	494	70.94		.617	4.44	13 1.	.00	36.57
			CA :	LEU	494	71.50		.637	2.57	1 1.	00	34.91
		771 (	CB p	LEU	494			344	2.90	_	00	36.04
AT	• ,	72 (			494	70.80		244	2.09		00	37.43
AT		73 c			494	71.312	2 0.	814	2.26	_	00	
AT	OM 37	_				71.327		437	3.73			36.62
ATO	OM 37	75 C			494	70.419	-0.	118	1.47	- •		36.37
ATO		_	_		494	72.967		451	2.51			40.70
ATO			~		194	73.308		160		_		37.08
ATO					195	73.839		779	1.560			34.90
ATC			_		195	75.246		330	3.243			37.18
ATO					95	75.885		066	2.918			39.84
ATO			A	LA 4	95	75.949			3.541			39.29
ATO		_	Al	ĹΑ 4	95	75.400	1.5		3.400		0	41.68
	_		GI	U 4	96	77.149	0.8		4.189			41.53
ATO	•		GI		96	77.936	1.3		2.881	1.0		13.44
ATO		6 CE	GI	_	96		0.2		3.297	1.0		12.86
ATO		7 CG			96	78.328	-0.6		2.101	1.0	_	4.63
ATOM	_	8 CD			96	77.120	-1.1		1.320	1.0		3.31
ATON					96	77.386	-2.4		0.545	1.00		
ATOM	1 379					76.494	-3.3		0.534	1.00		9.48
ATOM			GL			78.477	-2.5		0.053	1.00		2.39
ATOM		_				79.150	0.75		4.006			2.15
ATOM		-	GL			79.889	1.56		3.455	1.00		0.96
ATOM			AL		7	79.267	0.41			1.00		0.81
ATOM			AL		7	80.381	0.85		5.280	1.00		0.79
ATOM			ALA		7	79.888	1.24		.096	1.00		L.84
ATOM	,	•	ALA	49	7	81.394			478	1.00		3.80
		0	ALA	49	7	81.019	-0.28		.181	1.00		1.72
ATOM	3799	N	ILE	49	3	82.678	-1.44		.215	1.00		. 78
ATOM	3801	CA	ILE			83.729	0.05	_	.183	1.00		. 03
ATOM	3802	CB	ILE	498		D4 654	-0.95	26	. 255	1.00		.78
ATOM	3803	CG2	ILE	498		84.654	-0.89	4 5	.014	1.00		. 57
ATOM	3804	CG1	ILE	498		85.748	-1.954	4 5	.119	1.00		.32
ATOM	3805	CD1	ILE			83.851	-1.103		. 726	1.00		
ATOM	3806	C		498		83.139	0.146		198			. 90
ATOM	3807	Ö	ILE	498		84.573	-0.754		511	1.00		. 47
ATOM	3808		ILE	498		85.005	0.359			1.00	48.	
ATOM		N	GLY	499		84.754	-1.829		805	1.00	47.	
ATOM	3810	CA	GLY	499		35.563	-1.774		271	1.00	49.	
	3811	C	GLY	499		35.076				1.00	53.	
ATOM	3812	0	GLY	499		5.885	-0.944		657	1.00	57.	
ATOM	3813	N	LEU	500		3.768	-0.341	11.		1.00	59.	
ATOM	3815	CA	LEU	500			-0.948	10.	909	1.00	58.	
ATOM	3816	CB	LEU	500		3.193	-0.189	12.		1.00	57.	
				200	8	1.705	-0.519	12.		1.00	55.	
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MOTA	3817	CG	LEU	500	80.789	0.036	11.086	1.00	54.81
ATOM	3818	CD1	LEU	500	79.361	-0.445	11.293	1.00	53.00
ATOM	3819	CD2	LEU	500	80.854	1.561	11.089	1.00	53.27
MOTA	3820	С	LEU	500	83.926	-0.466	13.333	1.00	58.15
MOTA	3821	0	LEU	500	84.461	-1.560	13.529	1.00	60.29
MOTA	3822	N	PRO	505	87.397	-6.022	10.511	1.00	77.18
ATOM	3823	CD	PRO	505	88.509	-6.651	11.242	1.00	78.26
ATOM	3824	CA	PRO	505	87.755	-4.660	10.097	1.00	75.62
MOTA	3825	CB	PRO	505	89.166	-4.487	10.669	1.00	75.77
MOTA	3826	CG	PRO	505	89.696	-5.884	10.715	1.00	77.07
MOTA	3827	C	PRO	505	87.709	-4.440	8.583	1.00	73.15
MOTA	3828	0	PRO	505	87.772	-3.308	8.105	1.00	72.63
MOTA	3829	N	ASN	506	87.595	-5.524	7.830	1.00	71.27
MOTA	3831	CA	ASN	506	87.518	-5.421	6.380	1.00	69.14
ATOM	3832	CB	ASN	506	88.577	-6.313	5.728	1.00	70.76
ATOM	3833	C	ASN	506	86.119	-5.840	5.940	1.00	67.30
ATOM	3834	0	ASN	506	85.834	-5.957	4.750	1.00	67.03
MOTA	3835	N	ARG	507	85.250	-6.064	6.921	1.00	65.27
ATOM	3837	CA	ARG	507	83.876	-6.479	6.669	1.00	62.86
ATOM	3838	CB	ARG	507	83.335	-7.267	7.864	1.00	65.45
ATOM	3839	C	ARG	507	82.991	-5.274	6.443	1.00	59.56
ATOM	3840	0	ARG	507	83.161	-4.247	7.100	1.00	59.70
ATOM	3841	N	VAL	508	82.057	-5.397	5.509	1.00	56.65
ATOM	3843	CA	VAL	508	81.135	-4.310	5.226	1.00	55.48
ATOM	3844	CB	VAL	508	80.850	-4.157	3.719	1.00	55.71
ATOM	3845	CG1	VAL	508	82.146	-3.962	2.962	1.00	58.18
ATOM	3846	CG2	VAL	508	80.096	-5.356	3.188	1.00	58.76
ATOM	3847	С	VAL	508	79.833	-4.537	5.979	1.00	53.10
ATOM	3848	0	VAL	508	79.352	-5.665	6.091	1.00	54.25
ATOM	3849	N	THR	509	79.282	-3.460	6.514	1.00	50.06
ATOM	3851	CA	THR	509	78.041	-3.512	7.260	1.00	45.70
MOTA	3852	CB	THR	509	78.256	-3.029	8.715	1.00	45.59
MOTA	3853	OG1	THR	509	79.395	-3.696	9.279	1.00	43.86
MOTA	3855	CG2	THR	509	77.028	-3.328	9.573	1.00	44.19
ATOM	3856	C	THR	509	77.064	-2.574	6.564	1.00	43.57
ATOM	3857	0	THR	509	77.416	-1.444	6.221	1.00	41.15
MOTA	3858	N	LYS	510	75.871	-3.073	6.268	1.00	42.96
ATOM	3860	CA	LYS	510	74.847	-2.253	5.640	1.00	41.91
ATOM	3861	CB	LYS	510	73.740	-3.144	5.091	1.00	44.74
ATOM	3862	CG	LYS	510	72.864	-2.461	4.069	1.00	51.83
MOTA	3863	CD	LYS	510	73.392	-2.645	2.659	1.00	55.00
ATOM	3864	CE	LYS	510	72.769	-3.879	2.020	1.00	58.36
ATOM	3865	NZ	LYS	510	73.069	-5.131	2.769	1.00	58.57
ATOM	3869	С	LYS	510	74.322	-1.367	6.789	1.00	40.74
ATOM	3870	0	LYS	510	73.909	-1.874	7.837	1.00	40.26
ATOM	3871	N	VAL	511	74.413	-0.052	6.624	1.00	37.21
MOTA	3873	CA	VAL	511	73.989	0.877	7.661	1.00	33.44
MOTA	3874	СВ	VAL	511	75.227	1.515	8.362	1.00	
ATOM	3875	CG1	VAL	511	76.100	0.436	9.014	1.00	34.53 31.98
ATOM	3876	CG2	VAL	511	76.048	2.322	7.358	1.00	
ATOM	3877	C	VAL	511	73.134	1.989	7.338	1.00	34.82
ATOM	3878	0	VAL	511	73.134	2.130	5.871	1.00	31.34
ATOM	3879	N	ALA	512	72.485	2.748			31.33
ATOM	3881	CA	ALA	512			7.961	1.00	30.70
011	J J J J	CA.	ひたび	212	71.671	3.876	7.523	1.00	30.81

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		882	CB ;	ALA	512	70.30	)				
		883			512	72.45		0.2	-	00 29.85	
			_		512	73.03			04 1.	00 31.30	
	COM 3	885	N V		513	72.48					
		887	_		513		· -		99 1.		
		888		-	513	73.20				30.58	
		389 (			513	74.35					
AT		390 (			513	75.13	_				
AT	SE MO	391 (	~		13	75.29			23 1.0		
AT	BE MO	92 (		-	13	72.30			39 1.0	0 31.28	
ATO	38 MO	93 N	_		14	71.64			7 1.0		
ATO	38 MC	95 C			14	72.229			1.0		
ATO	OM 38		_		14	71.439					
ATC	38 MC		G L	_	14	70.881	_				
ATC	OM 38			-	14	69.977			6 1.0		
ATC	M 38				14	69.513		4 11.75			
ATO	M 39				14	68.514					
ATO	M 390					67.226					
ATO	M 390		LY			72.357					
ATO			ME			73.485	11.736				
ATO	M 390					71.867	12.580				
ATO	M 390					72.643	13.747				
ATO	M 391					73.435	13.442			30.64	
ATOM	4 391					72.557	13.038	4.464			
ATOM	4 391	2 CE				73.525	12.522			-2.10	
ATOM			MET			74.015	10.933				
ATOM	1 391		MET			71.675	14.869			29.71	
ATOM		5 ท	LEU			70.462	14.664		1.00	30.04	
ATOM	391	7 CA				72.212	16.060	6.445		29.56	
ATOM	3918	CB	LEU			71.381	17.206	6.136	1.00	30.76	
ATOM			LEU			72.093	18.508	6.526	1.00	28.20	
ATOM	3920	CD				72.396	18.724	8.011	1.00	28.48	
ATOM	3921	CD2				73.202	19.983	8.185	1.00	27.55	
ATOM	3922	C	LEU			71.114	18.814	8.794	1.00	25.49	
ATOM	3923	0	LEU	516		71.081	17.225	4.647	1.00	30.97	
ATOM	3924	N	LYS	517		71.728	16.534	3.851	1.00	29.93	
ATOM	3926	CA	LYS	517		70.030	17.946	4.291	1.00	31.57	
ATOM	3927	CB	LYS	517		69.677	18.117	2.899	1.00	31.44	
ATOM	3928		LYS	517		68.169	18.310	2.752	1.00	34.79	
ATOM	3929	CD	LYS	517		67.375	17.098	3.194	1.00	38.42	
ATOM	3930	CE	LYS	517		66.148 65.087	16.888	2.343	1.00	46.52	
ATOM	3931	NZ	LYS	517		63.901	17.950	2.582	1.00	53.77	
MOTA	3935	С	LYS	517		70.457	17.740	1.690	1.00	56.38	
ATOM	3936	0	LYS	517			19.377	2.499	1.00	30.18	
ATOM	3937	N	SER	518		70.892	20.134	3.370	1.00	27.47	
ATOM	3939	CA	SER	518		70.646	19.594	1.201	1.00	31.13	
ATOM	3940	CB	SER	518		71.394	20.747	0.693	1.00	32.11	
ATOM	3941	OG	SER	518		71.518	20.652	-0.824	1.00	33.45	
ATOM	3943	C	SER	518		70.242	20.567	-1.428	1.00	34.51	
ATOM	3944	0	SER	518		70.814	22.103	1.073	1.00	32.81	
ATOM	3945	N	ASP	519		71.515	23.123	1.027	1.00	34.03	
ATOM	3947	CA	ASP	519		69.540	22.117	1.449		29.80	
ATOM	3948	СВ	ASP	519		68.886	23.354	1.836		28.94	
ATOM	3949	CG	ASP	519		67.473	23.421	1.237	<b>-</b>	33.90	
		-		J 1 7	,	66.542	22.332	1.771		34 42	

66.542 22.332 1.771 1.00 34.42

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MOTA	3950	OD1	ASP	519	67.020	21.328	2.333	1.00	35.58
ATOM	3951	OD2	ASP	519	65.313	22.485	1.617	1.00	41.83
ATOM	3952	C	ASP	519	68.829	23.559	3.342	1.00	29.08
MOTA	3953	0	ASP	519	68.177	24.485	3.816	1.00	29.79
MOTA	3954	N	ALA	520	69.514	22.710	4.099	1.00	29.73
ATOM	3956	CA	ALA	520	69.488	22.824	5.558	1.00	29.16
MOTA	3957	CB	ALA	520	70.174	21.639	6.190	1.00	28.13
MOTA	3958	С	ALA	520	70.122	24.108	6.040	1.00	28.06
MOTA	3959	0	ALA	520	70.880	24.741	5.309	1.00	28.84
MOTA	3960	N	THR	521	69.800	24.491	7.272	1.00	27.84
ATOM	3962	CA	THR	521	70.357	25.692	7.885	1.00	30.45
MOTA	3963	CB	THR	521	69.254	26.635	8.463	1.00	33.56
ATOM	3964	OG1	THR	521	68.547	25.968	9.520	1.00	36.27
MOTA	3966	CG2	THR	521	68.275	27.074	7.379	1.00	36.06
ATOM	3967	C	THR	521	71.251	25.263	9.048	1.00	30.04
ATOM	3968	0	THR	521	71.348	24.072	9.369	1.00	28.16
MOTA	3969	N	GLU	522	71.876	26.241	9.696	1.00	31.42
MOTA	3971	CA	GLU	522	72.745	25.978	10.832	1.00	36.94
ATOM	3972	CB	GLU	522	73.404	27.282	11.299	1.00	44.74
ATOM	3973	CG	GLU	522	74.414	27.130	12.450	1.00	58.34
ATOM	3974	CD	GLU	522	75.769	26.579	12.009	1.00	64.50
ATOM	3975	OEl	GLU	522	76.798	27.261	12.231	1.00	64.89
ATOM	3976	OE2	GLU	522	75.806	25.461	11.452	1.00	70.26
ATOM	3977	С	GLU	522	71.932	25.345	11.969	1.00	34.02
MOTA	3978	0	GLU	522	72.428	24.480	12.684	1.00	31.11
ATOM	3979	N	LYS	523	70.670	25.750	12.097	1.00	32.53
MOTA	3981	CA	LYS	523	69.805	25.210	13.135	1.00	34.06
MOTA	3982	CB	LYS	523	68.481	25.970	13.188	1.00	39.54
MOTA	3983	CG	LYS	523	67.560	25.541	14.322	1.00	45.55
ATOM	3984	CD	LYS	523	66.360	24.776	13.789	1.00	52.08
ATOM	3985	CE	LYS	523	65.443	24.312	14.914	1.00	54.16
MOTA	3986	NZ	LYS	523	64.313	23.509	14.373	1.00	54.38
MOTA	3990	С	LYS	523	69.572	23.733	12.861	1.00	31.73
MOTA	3991	0	LYS	523	69.589	22.922	13.788	1.00	31.15
ATOM	3992	N	ASP	524	69.374	23.383	11.590	1.00	29.22
ATOM	3994	CA	ASP	524	69.182	21.980	11.214	1.00	28.79
ATOM	3995	CB	ASP	524	68.928	21.831	9.714	1.00	27.65
ATOM	3996	CG	ASP	524	67.586	22.396	9.286	1.00	33.89
MOTA	3997	OD1	ASP	524	66.568	22.106	9.954	1.00	34.66
MOTA	3998	OD2	ASP	524	67.549	23.120	8.270	1.00	30.04
ATOM	3999	C	ASP	524	70.424	21.190	11.606	1.00	28.00
ATOM	4000	0	ASP	524	70.317	20.104	12.162	1.00	30.83
ATOM	4001	N	LEU	525	71.603	21.761	11.347	1.00	29.87
ATOM	4003	CA	LEU	525	72.873	21.121	11.700	1.00	27.60
ATOM	4004	CB	LEU	525	74.064	21.997	11.282	1.00	24.08
ATOM	4005	CG	LEU	525	75.462	21.433	11.593	1.00	26.11
ATOM	4006	CD1	LEU	525	75.597	19.979	11.098	1.00	23.67
MOTA	4007	CD2	LEU	525	76.530	22.321	10.967	1.00	21.28
ATOM	4008	C	LEU	525	72.909	20.869	13.200	1.00	26.38
ATOM	4009	0	LEU	525	73.249	19.777	13.653	1.00	26.09
ATOM	4010	N	SER	526	72.560	21.902	13.956	1.00	29.72
ATOM	4012	CA	SER	526	72.500	21.861	15.422	1.00	32.16
ATOM	4013	CB	SER	526	71.980	23.209	15.939	1.00	33.45
ATOM	4014	OG	SER	526	71.793	23.213	17.343	1.00	40.42

ATOM 4017 O SER 526 71.572 20.728 15.902 1.00 31.64 ATOM 4018 N ASP 527 70.454 20.561 15.201 1.00 27.92 ATOM 4021 CB ASP 527 69.492 19.527 15.524 1.00 28.60 ATOM 4022 CG ASP 527 69.492 19.527 14.765 1.00 29.35 ATOM 4023 OD1 ASP 527 67.418 20.984 15.278 1.00 29.35 ATOM 4024 OD2 ASP 527 67.418 20.984 15.278 1.00 31.96 ATOM 4025 C ASP 527 66.456 21.369 16.353 1.00 31.96 ATOM 4026 O ASP 527 66.456 21.369 16.551 1.00 31.96 ATOM 4027 N LEU 528 70.721 15.246 1.00 29.555 ATOM 4030 CB LEU 528 71.302 16.652 13.794 1.00 29.555 ATOM 4031 CG LEU 528 71.302 16.658 13.794 1.00 29.565 ATOM 4030 CB LEU 528 71.302 16.658 13.794 1.00 29.565 ATOM 4031 CG LEU 528 71.302 16.658 13.794 1.00 29.565 ATOM 4032 CD LEU 528 71.780 16.621 12.336 1.00 28.32 ATOM 4033 CD LEU 528 71.780 16.621 12.336 1.00 28.32 ATOM 4034 C LEU 528 71.780 16.621 12.336 1.00 28.32 ATOM 4035 C LEU 528 72.450 14.189 12.035 1.00 27.72 ATOM 4036 C LEU 528 72.450 14.189 12.035 1.00 27.92 ATOM 4039 CB LEU 528 72.450 14.189 12.035 1.00 27.92 ATOM 4039 CB LEU 528 72.451 16.387 10.02 29.72 ATOM 4030 CB LEU 528 72.450 16.539 12.005 29.72 ATOM 4030 CB LEU 528 72.450 16.389 12.035 1.00 27.92 ATOM 4030 CB LEU 528 72.450 16.389 12.035 1.00 27.92 ATOM 4030 CB LEU 528 72.450 16.389 12.035 1.00 27.92 ATOM 4030 CB LEU 528 72.450 16.399 15.168 1.00 28.98 ATOM 4030 CB LEU 529 73.224 17.329 15.168 1.00 28.98 ATOM 4030 CB LEU 529 73.090 16.799 15.168 1.00 28.99 ATOM 4040 CG LEU 528 74.305 17.311 16.134 1.00 28.88 ATOM 4040 CG LEU 529 75.960 18.613 14.984 1.00 28.98 ATOM 4040 CG LEU 529 75.960 18.621 17.423 1.00 29.99 ATOM 4040 CG LEU 529 76.175 18.221 17.423 1.00 29.99 ATOM 4040 CG LEU 529 75.960 18.621 17.423 1.00 29.99 ATOM 4040 CG LEU 529 76.175 18.201 19.90 10.00 29.70 ATOM 4040 CG LEU 529 76.175 18.201 19.90 10.00 29.70 ATOM 4040 CG LEU 529 76.175 18.201 19.90 10.00 29.70 ATOM 4050 CB GUU 531 68.683 19.932 1.00 29.70 ATOM 4060 CB GUU 531 69.497 12.500 19.00 29.71 ATOM 4060 CB GUU 531 68.683 12.296 17.648 1.00 29.72 ATOM 4060 CB GUU 531 68.683 12.296 17.648 1.00 29.72 ATOM 4060 C	ATOM	4016	С										
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ATOM 4057 CG GLU 531 69.147 12.319 16.737 1.00 29.72  ATOM 4058 CD GLU 531 68.510 11.979 15.414 1.00 33.88  ATOM 4060 OE2 GLU 531 68.026 10.846 15.281 1.00 37.60  ATOM 4061 C GLU 531 71.578 12.974 18.271 1.00 28.91  ATOM 4063 N MET 532 72.686 13.179 17.567 1.00 29.46  ATOM 4066 CB MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4068 SD MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.732 14.400 16.117 1.00 24.10  ATOM 4071 O MET 532 74.948 12.280 19.078 1.00 24.10  ATOM 4071 O MET 532 74.948 13.454 19.681 1.00 29.74  ATOM 4070 CB GLU 533 74.481 13.454 19.681 1.00 29.74  ATOM 4070 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4070 CB GLU 533 75.182 15.008 21.423 1.00 29.66  ATOM 4070 CB GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4070 CB GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4070 CB GLU 533 76.331 15.687 20.651 1.00 32.23			GLU			70.458	1	3.999	18				
ATOM 4058 CD GLU 531 68.510 11.979 15.414 1.00 32.21  ATOM 4060 OE2 GLU 531 68.026 10.846 15.281 1.00 37.60  ATOM 4061 C GLU 531 71.578 12.974 18.271 1.00 28.91  ATOM 4062 O GLU 531 71.578 12.974 18.271 1.00 28.91  ATOM 4063 N MET 532 72.686 13.179 17.567 1.00 28.84  ATOM 4066 CB MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4066 CB MET 532 74.948 12.786 16.689 1.00 27.41  ATOM 4068 SD MET 532 77.503 12.675 15.640 1.00 32.27  ATOM 4069 CE MET 532 77.732 14.400 16.117 1.00 24.10  ATOM 4070 C MET 532 74.389 12.280 19.078 1.00 28.80  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 29.74  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 29.74  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4075 CB GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.00 34.47		7 CG				69.709	1.	3.727					
ATOM 4059 OE1 GLU 531 68.026 10.846 15.281 1.00 33.88  ATOM 4060 OE2 GLU 531 68.483 12.833 14.510 1.00 34.70  ATOM 4061 C GLU 531 71.578 12.974 18.271 1.00 28.91  ATOM 4063 N MET 532 72.686 13.179 17.567 1.00 28.84  ATOM 4066 CB MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4067 CG MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.503 12.675 15.640 1.00 32.27  ATOM 4070 C MET 532 77.732 14.400 16.117 1.00 24.10  ATOM 4071 O MET 532 74.389 12.280 19.078 1.00 24.10  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 29.74  ATOM 4074 CA GLU 533 74.985 13.546 21.033 1.00 29.74  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 34.47	7.000					69.147	12	2.319				-	
ATOM 4060 OE2 GLU 531 68.483 12.833 14.510 1.00 37.60  ATOM 4061 C GLU 531 71.578 12.974 18.271 1.00 34.70  ATOM 4063 N MET 532 72.686 13.179 17.567 1.00 29.46  ATOM 4066 CB MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4068 SD MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.503 12.675 15.640 1.00 22.27  ATOM 4070 C MET 532 74.389 12.280 19.078 1.00 24.10  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 29.74  ATOM 4074 CA GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4076 CG GLU 533 77.656 14.937 20.774		9 OE1				68.510	11	L. <b>9</b> 79					. 21
ATOM 4061 C GLU 531 71.578 12.974 18.271 1.00 34.70  ATOM 4062 O GLU 531 71.428 12.007 19.019 1.00 28.91  ATOM 4063 N MET 532 72.686 13.179 17.567 1.00 28.84  ATOM 4066 CB MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4067 CG MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.732 12.675 15.640 1.00 32.27  ATOM 4070 C MET 532 74.389 12.280 19.078 1.00 24.10  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 29.74  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 29.74  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.651 1.00 34.47						68.026			15.	281			
ATOM 4062 O GLU 531 71.428 12.974 18.271 1.00 28.91  ATOM 4063 N MET 532 72.686 13.179 17.567 1.00 29.46  ATOM 4066 CB MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4067 CG MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.503 12.675 15.640 1.00 32.27  ATOM 4070 C MET 532 74.389 12.280 19.078 1.00 24.10  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 29.74  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 29.74  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.00 34.47	•								14.	510			
ATOM 4063 N MET 532 72.686 13.179 17.567 1.00 29.46  ATOM 4066 CB MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4067 CG MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.503 12.675 15.640 1.00 32.27  ATOM 4070 C MET 532 74.389 12.280 19.078 1.00 24.10  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 29.74  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 28.83  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.00 34.47		2 0					12	. 974					
ATOM 4065 CA MET 532 73.851 12.296 17.648 1.00 29.35  ATOM 4066 CB MET 532 74.948 12.786 16.689 1.00 27.41  ATOM 4068 SD MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.503 12.675 15.640 1.00 32.27  ATOM 4070 C MET 532 74.389 12.280 19.078 1.00 24.10  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 29.74  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 28.83  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.00 34.47						71.428	12	.007	19.	019			
ATOM 4066 CB MET 532 74.948 12.786 16.689 1.00 29.35  ATOM 4068 SD MET 532 76.299 12.117 16.872 1.00 26.71  ATOM 4069 CE MET 532 77.503 12.675 15.640 1.00 32.27  ATOM 4070 C MET 532 74.389 12.280 19.078 1.00 24.10  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 28.80  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 28.83  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.20		CA				/2.686			17.	567		,	46
ATOM 4067 CG MET 532 76.299 12.117 16.872 1.00 27.41  ATOM 4068 SD MET 532 77.503 12.675 15.640 1.00 32.27  ATOM 4070 C MET 532 77.732 14.400 16.117 1.00 24.10  ATOM 4071 O MET 532 74.389 12.280 19.078 1.00 28.80  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 29.74  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.00 34.47									17.	648		-	84
ATOM 4068 SD MET 532 77.503 12.675 15.640 1.00 26.71  ATOM 4069 CE MET 532 77.732 14.400 16.117 1.00 24.10  ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 29.74  ATOM 4074 CA GLU 533 74.481 13.454 19.681 1.00 28.83  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774		CG				4.948	12	. 786					35
ATOM 4069 CE MET 532 77.732 14.400 16.117 1.00 32.27  ATOM 4071 C MET 532 74.389 12.280 19.078 1.00 28.80  ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 28.83  ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.20		SD				6.299	12.	.117				27.	41
ATOM 4070 C MET 532 77.732 14.400 16.117 1.00 24.10 ATOM 4071 O MET 532 74.700 11.230 19.630 1.00 28.80 ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 28.83 ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66 ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23 ATOM 4077 CD GLU 533 77.656 14.937 20.774		CE			7	7.503	12.	675					
ATOM 4071 O MET 532 74.700 11.230 19.078 1.00 28.80 ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 29.74 ATOM 4075 CB GLU 533 74.985 13.546 21.033 1.00 29.66 ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23 ATOM 4077 CD GLU 533 77.656 14.937 20.774					7	7.732	14.	400	16.1				
ATOM 4072 N GLU 533 74.481 13.454 19.681 1.00 28.80  ATOM 4074 CA GLU 533 74.985 13.546 21.033 1.00 29.66  ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23  ATOM 4077 CD GLU 533 77.656 14.937 20.774	ATOM 4071						12.	280					
ATOM 4074 CA GLU 533 74.481 13.454 19.681 1.00 28.83  ATOM 4075 CB GLU 533 75.182 15.008 21.423 1.00 29.66  ATOM 4077 CD GLU 533 76.331 15.687 20.651 1.00 32.23  77.656 14.937 20.774 1.00	ATOM 4072						11.	230					
ATOM 4075 CB GLU 533 75.182 15.008 21.423 1.00 29.66 ATOM 4076 CG GLU 533 76.331 15.687 20.651 1.00 32.23 ATOM 4077 CD GLU 533 77.656 14.937 20.774 1.00 34.47	T Const				7	4.481	13.	454					
ATOM 4076 CG GLU 533 75.182 15.008 21.423 1.00 29.66 ATOM 4077 CD GLU 533 76.331 15.687 20.651 1.00 32.23 77.656 14.937 20.774					7	4.985	13.	546	21 0				
ATOM 4077 CD GLU 533 76.331 15.687 20.651 1.00 32.23 77.656 14.937 20.774					7	5.182			21 4				
77.656 14.937 20.774 1 20.851	N CD				76	5.331			20 =				
			GTO	533	77	7.656							
	SSSD/55145. v0	1							~0.7	, a T	.00	38.0	3

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ATOM	4078	OE1	GLU	533	78.168	14.780	21.903	1.00	39.75	
ATOM	4079	OE2	GLU	533	78.192	14.497	19.736	1.00	38.75	
ATOM	4080	C	GLU	533	74.058	12.815	22.005	1.00	31.55	
ATOM	4081	0	GLU	533	74.521	12.083	22.889	1.00	30.63	
ATOM	4082	N	MET	534	72.750	12.958	21.799	1.00	31.31	
MOTA	4084	CA	MET	534	71.789	12.289	22.664	1.00	30.78	
ATOM	4085	CB	MET	534	70.348	12.672	22.319	1.00	31.23	
MOTA	4086	CG	MET	534	69.453	12.648	23.551	0.50	29.35 PRT1	
ATOM	4087	SD	MET	534	67.688	12.563	23.246	0.50	28.79 PRT1	
ATOM	4088	CE	MET	534	67.290	14.230	22.875	0.50	26.96 PRT1	
ATOM	4089	С	MET	534	71.991	10.773	22.560	1.00	28.82	
ATOM	4090	0	MET	534	72.053	10.083	23.568	1.00	30.10	
ATOM	4091	N	MET	535	72.149	10.271	21.339	1.00	29.16	
ATOM	4093	CA	MET	535	72.381	8.852	21.110	1.00	29.37	
ATOM	4094	CB	MET	535	72.546	8.551	19.617	1.00	27.35	
ATOM	4095	CG	MET	535	71.281	8.790	18.817	1.00	28.40	
ATOM	4096	SD	MET	535	71.255	7.955	17.255	1.00	30.26	
ATOM	4097	CE	MET	535	71.336	9.279	16.188	1.00	35.50	
ATOM	4098	С	MET	535	73.612	8.388	21.887	1.00	30.36	
ATOM	4099	0	MET	535	73.626	7.287	22.460	1.00	26.13	
ATOM	4100	И	LYS	536	74.640	9.233	21.909	1.00	30.70	
ATOM		CA	LYS	536	75.850	8.913	22.649	1.00	31.76	
MOTA		CB	LYS	536	76.934	9.954	22.388	1.00	31.05	
MOTA	4104	CG	LYS	536	77.550	9.883	21.004	1.00	26.80	
ATOM		CD	LYS	536	78.534	11.017	20.860	1.00	31.05	
MOTA		CE	LYS	536	79.132	11.138	19.466	1.00	29.83	
ATOM		NZ	LYS	536	79.957	12.377	19.440	1.00	29.32	
MOTA		С	LYS	536	75.550	8.834	24.150	1.00	31.99	
ATOM		0	LYS	536	75.920	7.859	24.806	1.00	31.92	
ATOM		N	MET	537	74.837	9.826	24.676	1.00	31.81	
ATOM		CA	MET	537	74.517	9.835	26.090	1.00	35.37	
ATOM		CB	MET	537	73.860	11.154	26.506	1.00	41.32	
MOTA		CG	MET	537	74.828	12.335	26.610	1.00	51.50	
ATOM		SD	MET	537	76.234	12.090	27.776	1.00	57.48	
ATOM		CE	MET	537	75.460	12.637	29.334	1.00	56.91	
ATOM		C	MET	537	73.630	8.679	26.499	1.00	36.11	
ATOM		0	MET	537	73.845	8.084	27.548	1.00	38.54	
ATOM	4122 4124	N	ILE ILE	538	72.652	8.347	25.661	1.00	33.69	
ATOM ATOM		CA		538	71.704	7.277	25.954	1.00	31.62	
ATOM		CB	ILE	538	70.492	7.314	24.974	1.00	28.21	
ATOM		CG2 CG1	ILE	538 538	69.681	6.013	25.034	1.00	28.22	
ATOM		CD1	ILE		69.590	8.488	25.338	1.00	23.74	
ATOM		CDI		538	68.487	8.728	24.344	1.00	27.94	
ATOM		0	ILE	538	72.322	5.894	26.008	1.00	31.07	
			ILE	538	71.952	5.080	26.860	1.00	33.13	
ATOM ATOM	4131	N	GLY	539	73.239	5.611	25.094	1.00	29.52	
	4133	CA	GLY	539	73.871	4.309	25.093	1.00	28.40	
ATOM	4134	C	GLY	539	73.111	3.275	24.289	1.00	30.21	
ATOM	4135	O N	GLY	539	72.018	3.554	23.788	1.00	29.66	
MOTA MOTA	4136 4138	N	LYS	540	73.679	2.074	24.199	1.00	28.44	
		CA	LYS	540	73.105	0.984	23.426	1.00	31.09	
ATOM ATOM	4139	CB	LYS	540	74.215	0.089	22.895	1.00	33.15	
ATOM		CG	LYS	540	75.116	0.776	21.906	1.00	39.54	
ATOM	4141	CD	LYS	540	76.125	-0.175	21.329	1.00	43.98	

		142 (	CE .	LYS	540	77.03				
		143 1		LYS	540	76.33	_			00 50.79
		147 (		LYS	540	72.05	_	· -		
AT	'OM 41	148.	_	LYS	540					
	OM 41	49 N	_	IIS	541	72.088			66 1.0	
AT	OM 41	51 (		iis	541	71.137			08 1.0	
AT	OM 41			IIS	541	70.080				
AT	OM 41		_	IIS	541	68.911		0 24.2		
ATO				IS		67.948		3 24.88		
ATO		-		IS	541	67.938		5 26.07		
ATO				IS	541	66.882		3 24.16		
ATC			_		541	66.268		7 24.88		0 32.95
ATC				IS	541	66.886		0 26.05		
ATO		_		IS	541	69.590	-2.01	3 22.34		-
ATO	-	-		IS	541	69.495	-1.40	4 21.27		
ATO		• •		rs •••	542	69.282	-3.309	22.47		
ATO					542	68.828	-4.133			
ATO					542	68.637	-5.587			
ATO			LY		542	67.560	-3.661			
ATO			LY		542	67.369	-3.903			
ATO			AS		543	66.683	-3.012			
ATON					543	65.425	-2.559			
ATON					543	64.245	-3.047			_
ATOM					543	64.253	-4.556			29.69
ATOM					543	64.510	-5.050			29.62
ATOM		_			543	64.020	-5.291	20.828		31.63
ATOM		_	ASI		543	65.299	-1.073	20.532		28.66
ATOM		-	ASI		543	64.207	-0.507	20.578		29.61
ATOM			IL	_	44	66.432	-0.442	20.222		28.00
ATOM			ILE		44	66.466	0.958	19.804	1.00	28.39
ATOM			ILE		44	66.903	1.952	20.935	1.00	25.73
ATOM					44	66.083	1.721	22.215	1.00	25.98
ATOM	4185			_	44	68.412	1.860	21.209	1.00	22.04 24.30
ATOM	4186				44	68.901	2.846	22.274	1.00	22.83
ATOM	4187	0	ILE	_	44	67.463	1.020	18.639	1.00	26.20
ATOM	4188	И	ILE	_	44	68.276	0.106	18.467	1.00	25.46
ATOM	4190	CA	ILE	_	45	67.307	2.016	17.771	1.00	26.26
ATOM	4191	CB	ILE ILE		45	68.223	2.209	16.641	1.00	27.62
ATOM	4192	CG2	ILE		15	67.647	3.195	15.585	1.00	28.33
ATOM	4193	CG1	ILE		15	68.726	3.595	14.562	1.00	28.00
ATOM	4194	CD1	ILE	54		66.453	2.565	14.856	1.00	24.69
ATOM	4195	C		54		66.850	1.467	13.875	1.00	26.17
ATOM	4196	o	ILE	54		69.492	2.794	17.267	1.00	28.23
ATOM	4197	N	ILE ASN	54		69.468	3.872	17.846	1.00	28.97
ATOM	4199	CA		54		70.595	2.069	17.164	1.00	29.45
ATOM	4200	CB	ASN	54		71.845	2.508	17.774	1.00	28.58
ATOM	4201	CG	ASN	54		72.580	1.309	18.384	1.00	
ATOM	4202	OD1	ASN	54		71.812	0.673	19.527		26.34 25.52
ATOM	4203		ASN	54		71.634	1.277	20.580		
ATOM	4206	ND2	ASN	54		71.341	-0.542	19.318		28.82
ATOM	4207	C	ASN	54		72.810		16.881		26.57
ATOM	4208	0	ASN	54		72.858		15.675		28.74
ATOM	4210	N	LEU	54	7	73.578		17.504		29.26
ATOM	4211	CA	LEU	54		74.618		16.834		29.90
		CB	LEU	547	7	75.075				30.27
SSD/ss	145 001							• • • •	00	25.85

AT	OM 4212	CG	LEU	547	76.161	7.034	17.232	1.00	27.73
AT	OM 4213	CD1	LEU	547	75.670	7.851	16.033	1.00	27.38
AT	OM 4214	CD2	LEU	547	76.545	7.966	18.345	1.00	29.14
AT	OM 4215	C	LEU	547	75.811	4.004	16.567	1.00	32.22
AT	OM 4216	0	LEU	547	76.256	3.291	17.471	1.00	33.38
AT	OM 4217	N	LEU	548	76.317	4.005	15.335	1.00	32.12
AT	OM 4219	CA	LEU	548	77.452	3.159	14.960	1.00	32.94
ATO	OM 4220	СВ	LEU	548	77.103	2.310	13.740	1.00	29.97
ATO	OM 4221	CG	LEU	548	75.839	1.458	13.840	1.00	31.55
ATO	OM 4222	CD1	LEU	548	75.662	0.713	12.540	1.00	27.85
ATO	OM 4223	CD2	LEU	548	75.917	0.500	15.025	1.00	
ATO	OM 4224	С	LEU	548	78.726	3.955	14.654	1.00	36.06
ATO	OM 4225	0	LEU	548	79.836	3.410	14.668	1.00	36.42
ATO	OM 4226	N	GLY	549	78.562	5.219	14.298	1.00	35.78
ATO	OM 4228	CA	GLY	549	79.713	6.042	13.987	1.00	36.22
ATO			GLY	549	79.267	7.376	13.433	1.00	35.30
ATO	OM 4230	0	GLY	549	78.062	7.646	13.362	1.00	33.46
ATO	OM 4231	N	ALA	550	80.232	8.206	13.042	1.00	34.94
ATO	OM 4233	CA	ALA	550	79.945	9.525	12.490	1.00	31.91
ATO	OM 4234	CB	ALA	550	79.588	10.495	13.613	1.00	30.54
ATO	OM 4235	С	ALA	550	81.128	10.077	11.715	1.00	31.58
ATO	OM 4236	0	ALA	550	82.281	9.832	12.080	1.00	31.23
ATO			CYS	551	80.818	10.812	10.643	1.00	31.13
ATC	OM 4239		CYS	551	81.805	11.503	9.804	1.00	28.28
ATC		CB	CYS	551	81.621	11.180	8.316	1.00	27.27
ATC		SG	CYS	551	81.771	9.449	7.839	1.00	30.33
ATC	M 4242	С	CYS	551	81.450	12.960	10.074	1.00	25.88
ATC	M 4243	0	CYS	551	80.432	13.458	9.605	1.00	27.73
ATC	M 4244	N	THR	552	82.214	13.586	10.954	1.00	25.35
ATC	OM 4246	CA	THR	552	81.988	14.967	11.353	1.00	26.79
ATC	M 4247	CB	THR	552	82.051	15.092	12.899	1.00	27.76
ATC	M 4248	OG1	THR	552	83.392	14.839	13.338	1.00	27.62
ATC	M 4250	CG2	THR	552	81.119	14.086	13.575	1.00	29.17
ATC	M 4251	С	THR	552	83.036	15.931	10.790	1.00	25.03
ATC	M 4252	0	THR	552	82.825	17.137	10.746	1.00	25.34
ATC	M 4253	N	GLN	553	84.174	15.385	10.381	1.00	27.34
ATC	M 4255	CA	GLN	553	85.285	16.190	9.888	1.00	26.31
ATC	M 4256	CB	GLN	553	86.601	15.639	10.468	1.00	25.05
ATC	M 4257	CG	GLN	553	86.581	15.491	11.993	1.00	24.78
ATO	M 4258	CD	GLN	553	86.382	16.823	12.709	1.00	25.40
ATO	M 4259	OE1	GLN	553	87.175	17.748	12.546	1.00	33.74
ATO	M 4260	NE2	GLN	553	85.338	16.920	13.516	1.00	25.61
ATO	M 4263	C	GLN	553	85.390	16.274	8.379	1.00	27.08
ATO	M 4264	0	GLN	553	85.083	15.318	7.669	1.00	28.76
ATO	M 4265	N	ASP	554	85.804	17.438	7.899	1.00	28.63
ATO	M 4267	CA	ASP	554	86.015	17.677	6.471	1.00	29.70
ATO	M 4268	·CB	ASP	554	87.335	17.050	6.051	1.00	29.73
ATO	M 4269	CG	ASP	554	88.480	17.587	6.857	1.00	33.38
ATO	M 4270	OD1	ASP	554	88.794	18.780	6.711	1.00	36.53
ATO	M 4271	OD2	ASP	554	89.024	16.841	7.687	1.00	36.40
ATO	M 4272	С	ASP	554	84.908	17.258	5.522	1.00	29.64
ATO		0	ASP	554	85.112	16.422	4.643	1.00	32.06
ATO	M 4274	N	GLY	555	83.748	17.881	5.679	1.00	28.59
ATO		CA	GLY	555	82.620	17.579	4.825	1.00	26.85
				_					



ATO		77 C	GL	Y 555	81.333	3 17.43	4 5 60		
ATO		_	GL	Y 555	81.319				
ATO		79 N	PR	0 556	80.229			_	50
ATO	M 428	0 CD	PR	0 556	80.159				
ATO		1 CA	PR	0 556	78.920				
ATO	M 428	2 CB	PRO	0 556	78.033				20
ATO		3 CG	PRO		79.025	_			23.37
ATO	M 428	4 C	PRO		78.885				24.44
ATOM	M 428	5 0	PRO		79.515				26.50
ATON	428	6 N	LEC		78.171				27.38
ATON	428	8 CA	LEU		78.032	16.314		-	26.25
ATOM	428	9 CB	LEU		77.403	15.452			28.25
ATOM	1 429	O CG	LEU	_	76.922	16.217			27.09
ATOM	1 429	CD:			78.088	15.414		1.00	28.35
ATOM	4292			-		14.733		1.00	25.54
ATOM	4293		LEU		76.204	16.340	12.271	1.00	26.91
ATOM	4294		LEU		77.169	14.246	8.554	1.00	29.06
ATOM			TYR		76.060	14.385	8.011	1.00	29.05
ATOM	4297		TYR		77.717	13.065	8.807	1.00	29.43
ATOM			TYR		77.018	11.823	8.573	1.00	28.02
ATOM			TYR	558	77.813	10.918	7.632	1.00	27.83
ATOM	4300			558	77.969	11.414	6.203	1.00	31.70
ATOM				558	78.966	10.893	5.383	1.00	32.90
ATOM	4302		TYR		79.121	11.315	4.073	1.00	32.69
MOTA	4303		TYR	558	77.122	12.386	5.666	1.00	30.23
ATOM	4304	CZ	TYR	558 550	77.271	12.815	4.350	1.00	29.97
ATOM	4305	OH	TYR	558	78.280	12.272	3.560	1.00	33.20
MOTA	4307	C		558	78.452	12.681	2.253	1.00	35.32
ATOM	4308	0	TYR	558	76.848	11.131	9.932	1.00	28.42
ATOM	4309	Ŋ	TYR	558	77.823	10.902	10.647	1.00	27.81
ATOM	4311	CA	VAL	559	75.601	10.870	10.313	1.00	29.20
ATOM	4312	CB	VAL	559	75.286	10.175	11.564	1.00	29.17
ATOM	4313	CG1	VAL	559	74.102	10.832	12.329	1.00	28.53
ATOM	4314	CG2	VAL	559	73.802	10.036	13.607	1.00	27.08
ATOM	4315	C	VAL	559	74.456	12.281	12.687	1.00	23.27
ATOM	4316		VAL	559	74.911	8.772	11.137	1.00	26.41
ATOM	4317	O N	VAL	559	73.834	8.536	10.593		25.91
ATOM	4319	N Ca	ILE	560	75.824	7.846	11.371		26.71
ATOM	4320	CA CB	ILE	560	75.638	6.465	10.966	_	27.55
ATOM	4321		ILE	560	77.012	5.829	10.619	_	28.48
ATOM	4322	CG2	ILE	560	76.819	4.468	9.979		29.18
ATOM	4323	CG1	ILE	560	77.793	6.745	9.657		27.99
ATOM	4324	CD1	ILE	560	79.274	6.399	9.525		28.97
ATOM		C	ILE	560	74.917	5.644	12.034		29.17
ATOM	4325	0	ILE	560	75.404	5.497	13.160		28.92
ATOM	4326	N	LAV	561	73.743	5.129			
ATOM	4328	CA	VAL	561	72.957	4.325			28.60 28.58
	4329	CB	VAL	561	71.634	5.061			
ATOM	4330	CG1	VAL	561	71.951	6.400		_	27.53
ATOM	4331	CG2	VAL	561	70.697	5.246			22.44
ATOM	4332	C	VAL	561	72.618	2.956			23.19
ATOM	4333	0	VAL	561	72.875				8.20
ATOM	4334	N	GLU	562	72.057			_	7.99
	4336	CA	GLU	562	71.666				9.17
ATOM	4337	CB	GLU	562	71.199				8.96
						J. 006	13.589	1.00 2	7.34

ATOM	4338	CG	GLU	562	72.308	-0.331	14.583	1.00	30.12
ATOM	4339	CD	GLU	562	71.838	-1.075	15.808	1.00	32.29
ATOM	4340	OE1	GLU	562	72.526	-2.030	16.217	1.00	32.45
ATOM	4341	OE2	GLU	562	70.785	-0.702	16.362	1.00	30.16
ATOM	4342	С	GLU	562	70.580	0.794	11.340	1.00	29.79
ATOM	4343	0	GLU	562	69.690	1.653	11.386	1.00	29.75
MOTA	4344	N	TYR	563	70.684	-0.106	10.369	1.00	30.51
MOTA	4346	CA	TYR	563	69.735	-0.209	9.267	1.00	33.76
ATOM	4347	CB	TYR	563	70.494	-0.602	7.988	1.00	31.04
ATOM	4348	CG	TYR	563	69.624	-0.928	6.806	1.00	33.40
MOTA	4349	CD1	TYR	563	68.693	-0.019	6.340	1.00	33.07
ATOM	4350	CE1	TYR	563	67.908	-0.301	5.240	1.00	34.71
ATOM	4351	CD2	TYR	563	69.749	-2.141	6.147	1.00	34.61
ATOM	4352	CE2	TYR	<b>56</b> 3	68.970	-2.446	. 5.035	1.00	36.54
ATOM	4353	CZ	TYR	563	68.047	-1.518	4.589	1.00	36.83
ATOM	4354	OH	TYR	563	67.261	-1.805	3.501	1.00	38.81
ATOM	4356	C	TYR	563	68.655	-1.269	9.588	1.00	36.14
MOTA	4357	0	TYR	563	68.946	-2.365	10.023	1.00	37.70
MOTA	4358	N	ALA	564	67.406	-0.948	9.309	1.00	37.87
MOTA	4360	CA	ALA	564	66.276	-1.832	9.534	1.00	38.49
ATOM	4361	CB	ALA	564	65.278	-1.167	10.458	1.00	42.57
MOTA	4362	C	ALA	564	65.645	-2.153	8.179	1.00	39.65
MOTA	4363	0	ALA	564	64.796	-1.423	7.687	1.00	39.74
MOTA	4364	N	SER	565	66.039	-3.280	7.607	1.00	40.06
MOTA	4366	CA	SER	565	65.567	3.699	6.295	1.00	40.67
MOTA	4367	CB	SER	565	66.267	-4.986	5.883	1.00	38.71
ATOM	4368	OG	SER	565	66.107	-5.964	6.889	1.00	41.35
ATOM	4370	С	SER	565	64.081	-3.884	6.106	1.00	42.17
ATOM	4371	0	SER	565	63.585	-3.741	4.992	1.00	44.25
MOTA	4372	N	LYS	566	63.360	-4.207	7.167	1.00	41.71
MOTA	4374	CA	LYS	566	61.928	-4.427	7.015	1.00	40.22
MOTA	4375	CB	LYS	566	61.525	-5.668	7.800	1.00	39.51
MOTA	4376	CG	LYS	566	62.202	-6.910	7.226	1.00	41.48
ATOM	4377	CD	LYS	566	62.113	-8.094	8.149	1.00	41.53
MOTA	4378	CE	LYS	566	62.710	-9.312	7.491	1.00	41.18
ATOM	4379	NZ	LYS	566	62.763	-10.458	8.438	1.00	46.17
ATOM ATOM	4383 4384	С О	LYS LYS	566 566	61.007	-3.220	7.263	1.00	40.47
ATOM	4385	N	GLY		59.800	-3.367	7.486	1.00	42.68
ATOM				567 563	61.584	-2.026	7.167		38.90
ATOM	4387 4388	CA C	GLY GLY	567 567	60.826	-0.799	7.336	1.00	37.13
ATOM	4389	0	GLY	567	60.199 60.644	-0.592 -1.172	8.694 9.683	1.00	36.72
ATOM	4390	N	ASN	568	59.191	0.273	8.753	1.00	38.48 35.77
ATOM	4392	CA	ASN	568	58.518	0.549	10.015	1.00	35.36
ATOM	4393	CB	ASN	568	57.883	1.957	10.015	1.00	36.30
ATOM	4394	CG	ASN	568	56.635	2.088	9.169	1.00	38.06
ATOM	4395	OD1	ASN	568	55.623	1.421	9.383	1.00	38.66
ATOM	4396	ND2	ASN	568	56.686	3.010	8.221	1.00	37.29
ATOM	4399	C	ASN	568		-0.532	10.341		
ATOM	4400	0	ASN	568	57.504 57.061		9.461	1.00 1.00	33.04
ATOM	4401	N	LEU	569	57.142	-1.265 -0.612	11.617	1.00	32.10 33.59
ATOM	4403	CA	LEU	569	56.199	-1.604	12.132	1.00	32.91
ATOM	4404	CB	LEU	569	56.045	-1.428	13.647	1.00	33.84
ATOM	4405	CG	LEU	569	55.088	-2.343	14.403	1.00	31.96
					JJ.000	2.343	74.40J	1.00	J I . J U





ATOM 4406 CD1 LEU 569 55.522 -3.797 14.216 1.00 33.20 ATOM 4407 CD2 LEU 569 55.089 -1.967 15.868 1.00 30.81 ATOM 4408 C LEU 569 54.820 -1.591 11.478 1.00 32.12 ATOM 4409 0 LEU 569 54.214 -2.645 11.300 1.00 33.08 MOTA 4410 N ARG 570 54.315 -0.409 11.148 1.00 32.05 MOTA 4412 CA ARG 570 52.999 -0.293 10.529 1.00 35.21 **ATOM** 4413 CB ARG 570 52.659 1.173 10.256 1.00 36.77 ATOM 4414 CG ARG 570 51.282 1.370 9.653 1.00 43.11 ATOM 4415 CD ARG 570 51.203 2.690 8.926 1.00 49.24 MOTA 4416 NE ARG 570 52,154 2.775 7.815 1.00 55.77 ATOM 4418 CZARG 570 52.995 3.790 7.619 1.00 58.89 MOTA 4419 NH1 ARG 570 53.016 4.820 8.463 1.00 61.61 MOTA 4422 NH2 ARG 570 53.804 3.786 6.566 1.00 59.16 ATOM 4425 C **ARG** 570 52.992 -1.063 9.220 1.00 35.16 MOTA 4426 0 ARG 570 52.145 -1.922 8.990 1.00 35.50 **ATOM** 4427 N GLU 571 53.971 -0.760 8.383 1.00 36.29 MOTA 4429 CA GLU 571 54.111 -1.400 7.089 1.00 37.51 **ATOM** 4430 CB GLU 571 55.219 -0.701 6.308 41.27 1.00 ATOM 4431 CG GLU 571 54.945 0.778 6.110 1.00 49.88 ATOM 4432 CD GLU 571 56.087 1.516 5.436 1.00 57.58 **ATOM** 4433 OE1 GLU 571 57.264 1.122 5.636 1.00 60.59 **ATOM** 4434 OE2 GLU 571 55.804 2.504 4.714 1.00 61.14 MOTA 4435 Ç GLU 571 54.399 -2.896 7.228 1.00 36.24 ATOM 4436 O GLU 571 53.889 -3.716 6.459 1.00 34.22 ATOM 4437 N TYR 572 55.202 -3.238 8.232 1.00 35.98 **ATOM** 4439 CA TYR 572 55.570 -4.619 8.517 1.00 35.34 ATOM 4440 CB TYR 572 56.526 -4.656 9.714 1.00 30.94 ATOM 4441 CG TYR 572 56.959 -6.034 10.180 1.00 32.71 **ATOM** 4442 CD1 TYR 572 58.009 -6.714 9.547 1.00 32.33 MOTA 4443 CE1 TYR 572 58.464 -7.940 10.026 1.00 30.31 MOTA 4444 CD2 TYR 572 56.369 -6.626 11.303 1.00 33.43 MOTA 4445 CE2 TYR 572 56.813 -7.851 11.791 1.00 31.46 MOTA 4446 CZTYR 572 57.864 -8.502 11.148 1.00 33.99 ATOM. 4447 OH TYR 572 58.311 -9.706 11.640 1.00 36.30 **ATOM** 4449 C TYR 572 54.312 -5.425 8.826 1.00 37.26 **ATOM** 4450 0 TYR 572 54.121 -6.530 8.314 1.00 36.91 ATOM 4451 N LEU 573 53.457 -4.850 9.665 1.00 36.82 ATOM 4453 CA LEU 573 52.208 -5.476 10.075 1.00 35.56 ATOM 4454 CB LEU 573 51.537 -4.629 11.165 1.00 34.03 ATOM 4455 CG LEU 573 52.238 -4.527 12.519 1.00 32.82 MOTA 4456 CD1 LEU 573 51.621 -3.423 13.377 1.00 28.95 **ATOM** 4457 CD2 LEU 573 52.168 -5.858 13.207 1.00 29.46 ATOM 4458 С LEU 573 51.237 -5.658 8.915 1.00 34.56 **ATOM** 4459 0 LEU 573 50.670 -6.729 8.726 1.00 34.80 ATOM 4460 N GLN 574 51.030 -4.602 8.150 1.00 37.10 ATOM 4462 CA GLN 574 50.101 -4.666 7.031 1.00 41.15 ATOM 4463 CB GLN 574 49.875 -3.278 6.457 1.00 41.63 ATOM 4464 CG GLN 574 49.089 -2.375 7.366 1.00 43.13 **ATOM** 4465 CD GLN 574 49.063 -0.959 6.860 1.00 47.77 MOTA 4466 OE1 GLN 574 49.655 -0.647 5.827 1.00 50.00 ATOM 4467 NE2 GLN 574 48.378 -0.086 7.582 1.00 49.67 MOTA 4470 C GLN 574 50.529 -5.627 5.934 1.00 42.38 ATOM 4471 0 GLN 574 49.685 -6.284 5.318 1.00 44.56

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4472

N

ALA

575

51.835

-5.717

5.697

1.00

41.99

ATOM

MOTA	4474	CA	ALA	575	52.367	-6.608	4.676	1.00	41.29
MOTA	4475	CB	ALA	575	53.841	-6.325	4.446	1.00	40.43
ATOM	4476	C	ALA	575	52.186	-8.058	5.066	1.00	41.42
MOTA	4477	0	ALA	575	52.392	-8.949	4.249	1.00	43.65
MOTA	4478	N	ARG	576	51.815	-8.294	6.319	1.00	42.56
MOTA	4480	CA	ARG	576	51.642	-9.646	6.824	1.00	42.51
ATOM	4481	CB	ARG	576	52.676	-9.910	7.920	1.00	40.14
ATOM	4482	CG	ARG	576	54.100	-9.896	7.377	1.00	40.32
ATOM	4483	CD	ARG	576	55.172	-9.836	8.460	1.00	40.78
MOTA	4484	NE	ARG	576	56.513	-9.783	7.874	1.00	42.13
MOTA	4486	CZ	ARG	576	56.975	-8.785	7.120	1.00	40.73
MOTA	4487	NH1	ARG	576	56.215	-7.732	6.851	1.00	39.21
ATOM	4490	NH2	ARG	576	58.201	-8.846	6.622	1.00	37.62
ATOM	4493	C	ARG	576	50.242	-9.931	7.326	1.00	44.48
MOTA	4494	0	ARG	576	50.028	-10.869	8.098	1.00	46.84
ATOM	4495	N	ARG	577	49.275	-9.146	6.866	1.00	46.26
ATOM	4497	CA	ARG	577	47.893	-9.344	7.292	1.00	46.89
ATOM	4498	CB	ARG	57 <b>7</b>	47.027	-8.170	6.845	1.00	46.16
MOTA	4499	CG	ARG	577	47.189	-6.939	7.696	1.00	44.93
MOTA	4500	CD	ARG	577	46.463	-5.766	7.080	1.00	44.60
MOTA	4501	NE	ARG	577	46.284	-4.683	8.039	1.00	45.05
MOTA	4503	CZ	ARG	577	45.612	-3.565	7.793	1.00	45.95
ATOM	4504	NH1	ARG	577	45.052	-3.372	6.606	1.00	47.39
MOTA	4507	NH2	ARG	577	45.466	-2.655	8.749	1.00	45.49
ATOM	4510	C	ARG	577	47.334	-10.649	6.740	1.00	46.60
ATOM	4511	0	ARG	577	47.478	-10.933	5.551	1.00	47.15
ATOM	4512	N	GLN	594	53.312	-14.007	7.967	1.00	63.97
MOTA	4514	CA	GLN	594	52.110	-14.068	8.799	1.00	63.06
MOTA	4515	CB	GLN	594	51.175	-15.183	8.319	1.00	64.16
ATOM	4516	C	GLN	594	52.501	-14.278	10.258	1.00	61.68
MOTA	4517	0	GLN	594	53.101	-15.292	10.619	1.00	60.95
MOTA	4518	N	LEU	595	52.140	-13.313	11.092	1.00	58.58
MOTA	4520	CA	LEU	595	52.470	-13.335	12.505	1.00	55.58
ATOM	4521	CB	LEU	595	52.619	-11.902	13.020	1.00	54.05
ATOM	4522	CG	LEU	595	53.570	-11.074	12.153	1.00	56.23
ATOM	4523	CD1	LEU	595	53.496	-9.609	12.524	1.00	58.84
ATOM	4524	CD2	LEU	595	54.977	-11.596	12.301	1.00	55.93
ATOM	4525	C O	LEU	595	51.480	-14.093	13.372	1.00	53.77
MOTA	4526	-	LEU	595	50.276	-14.046	13.139	1.00	54.31
MOTA	4527	N	SER	596	52.012	-14.780	14.377	1.00	51.04
ATOM	4529	CA	SER	596 506	51.206	-15.541	15.316	1.00	48.97
ATOM	4530	CB	SER	596	52.004	-16.737	15.834	1.00	48.89
ATOM	4531	og G	SER	596	52.945	-16.345	16.820	1.00	48.59
ATOM ATOM	4533	C	SER	596	50.853	-14.641	16.488	1.00	47.56
ATOM	4534	0	SER	596	51.470	-13.590	16.676	1.00	46.71
	4535	N	SER	597	49.888	-15.070	17.292	1.00	47.11
MOTA	4537	CA	SER	597	49.462	-14.315	18.461	1.00	47.88
ATOM ATOM	4538	CB	SER	597 597	48.386	-15.084	19.229	1.00	50.66
	4539	OG C	SER	597 597	47.574	-15.839	18.343	1.00	57.08
ATOM	4541	C	SER	597	50.666	-14.068	19.372	1.00	46.03
ATOM	4542	0	SER	597	50.735	-13.045	20.047	1.00	46.49
ATOM	4543	N C2	LYS	598 500	51.607	-15.007	19.399	1.00	46.08
ATOM ATOM	4545 4546	CA	LYS	598 598	52.798	-14.844	20.229	1.00	46.33
ATOM	4546	CB	LYS	598	53.558	-16.163	20.384	1.00	46.67

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	ATOM	4547	CG		_									
	<b>-</b>	4548	CD	LYS	598	54.4	49	-16.	224	21.623				
		4549	CE	LYS	598	55.2	40	-17.			-	_	9.61	
		4550	NZ	LYS	598	55.8	99	-17.		21.668			3.69	
		1554		LYS	598	54.89	91	-18.	_	3.026			3.15	
		1555	C	LYS	598	53.7(		-13.		4.093	1.00	52	.02	
				LYS	598	54.29		-12.9	_	9.599	1.00	45	.43	
		556		ASP	599	53.78		-13.8		0.311	1.00	44	.18	
		558		ASP	599	54.59				8.264	1.00		.16	
		559		ASP	599	54.52		-12.8		7.513	1.00		. 46	
	_	560		ASP	599	55.28		13.0		5.001	1.00		. 83	
			OD1 /	ASP	599	56.22		14.3	-	5.560	1.00		24	
			OD2 1	ASP	599	54.95		14.7		.260	1.00		90	
			C p		599	54.12		14.8		.493	1.00	51.		
			0 2	_	599	54.12(		11.4		.796	1.00	42.		
	OM 45	65 <u>1</u>			600	54.937		10.5		.059	1.00	45.		
		67 (	CA L		500	52,803		11.23		.776	1.00			
		68 (		_	500	52.246		-9.91	.8 18	.030	1.00	37.		
		69 C		`	500	50.747		9.88		.747	1.00	34.		
AT		70 C			00	50.332	- 1	10.06		. 281	1.00	34.		
ATO		71 C	_	~	00	48.814	-	9.99	2 16.	190	1.00	33.		
ATO		72 C			00	50.974	-	9.01			1.00	37.		
ATO		73 0				52.537	-	9.45			1.00	25.6		
ATC	DM 457	74 N		-	00 01	52.910	-	8.29	4 19.	_	1.00	34.5		
ATC			• •	-		52.415	-1	0.348				33.1		
ATO		'7 CI			01	52.692		9.969		_	1.00	34.2	4	
ATO	M 457				01	52.214	-1:	1.036	22.		1.00	35.8		
ATO						52.331	-10	0.483			1.00	37.5		
ATO	M 458		VA:			50.766	-11	409	22.			38.0		
ATO	M 458		VAI			54.198		741				40.7		
ATO		_	SER			54.634		.856				35.04		
ATOM	4 4584					54.981	-10	. 531	21.2			34.3		
MOTA	1 4585					56.421	-10	.421	21.3			32.58		
ATOM			SER			57.045	-11	. 504	20.4			36.01		
ATOM	1 4588		SER			58.453		.387	20.4			88.43		
ATOM		_	SER			56.809		. 038	20.8			3.36		
ATOM			SER			57.651		. 363	21.3			5.21		
ATOM			CYS	603		56.183		614	19.70		.00 3	5.03		
ATOM			CYS	603		56.438		294				4.15		
ATOM	4594	SG	CYS	603		55.543		055	19.14			4.04		
ATOM	4595		CYS	603		55.653		423	17.92			3.45		
ATOM	4596	C	CYS	603		56.198		211	17.22		50 3:	2.19	PRT1	
ATOM	4597	0	CYS	603		57.023.		316	20.19	_	00 32	2.79		
ATOM	4599	N	ALA	604	9	55.088	-6.		20.36			.36		
ATOM		CA	ALA	604	9	54.743			20.91		00. 31	31		
ATOM	4600	CB	ALA	604	9	3.321	-5.3	- J G	21.96		00 32	.36		
ATOM	4601	С	ALA	604	5	5.741	-5.6	5 T O	22.48			.01		
	4602	0	ALA	604	5	6.050	-5.3	594	23.12	3 1.0		.83		
ATOM	4603	N	TYR	605	5	6.212	-4.3	58	23.72	7 1.0		.89		
ATOM	4605	CA	TYR	605	5		-6.5		23.465	1.0		. 95		
ATOM	4606	CB	TYR	605	5	_	-6.7		24.539	1.0		. 34		
ATOM	4607	CG	TYR	605	5	_	-8.2		24.737	1.0	_	. 58		٠
ATOM	4608	CD1	TVP	605	<b>5</b>	0.040	-8.4	95	25.690	1 0				

58.511

59.556

59.841

60.896

-8.495 25.690

27.053

27.943

25.230

26.109

-8.236

-8.507

-9.026

-9.300

1.00

1.00

1.00

1.00

1.00

32.51

33.50

37.08

34.22

36.64

SSSD/55145. v01

4608 CD1

4610 CD2

CE1

CE2

4609

4611

TYR

TYR

TYR

TYR 605

605

605

605

ATOM

ATOM

ATOM



ATOM	4612	CZ	TYR	605	60.746	-9.042	27.464	1.00	37.56
ATOM	4613	OH	TYR	605	61.776	-9.342	28.336	1.00	38.08
MOTA	4615	С	TYR	605	58.480	-6.006	24.191	1.00	32.42
MOTA	4616	0	TYR	605	58.975	-5.203	24.991	1.00	33.34
MOTA	4617	N	GLN	606	58.997	-6.267	22.989	1.00	30.61
MOTA	4619	CA	GLN	606	60.218	-5.643	22.474	1.00	31.12
ATOM	4620	CB	GLN	606	60.499	-6.143	21.058	1.00	30.57
MOTA	4621	CG	GLN	606	61.044	-7.568	21.008	1.00	33.90
MOTA	4622	CD	GLN	606	61.240	-8.080	19.593	1.00	32.17
MOTA	4623	OE1	GLN	606	62.155	-7.652	18.883	1.00	32.55
MOTA	4624	NE2	GLN	606	60.374	-8.998	19.171	1.00	33.10
MOTA	4627	C	GLN	606	60.157	-4.114	22.487	1.00	31.69
MOTA	4628	0	GLN	606	61.111	-3.453	22.910	1.00	31.18
MOTA	4629	N	VAL	607	59.035	-3.564	22.020	1.00	29.50
MOTA	4631	CA	VAL	607	58.816	-2.122	22.000	1.00	27.54
ATOM	4632	CB	VAL	607	57.454	-1.751	21.306	1.00	26.79
ATOM	4633	CG1	VAL	607	57.131	-0.291	21.516	1.00	24.80
MOTA	4634	CG2	VAL	607	57.505	-2.050	19.815	1.00	22.95
MOTA	4635	C	VAL	607	58.827	-1.576	23.432	1.00	28.30
MOTA	4636	0	VAL	607	59.469	-0.548	23.705	1.00	28.32
MOTA	4637	N	ALA	608	58.110	-2.247	24.340	1.00	27.21
MOTA	4639	CA	ALA	608	58.061	-1.805	25.735	1.00	26.54
ATOM	4640	CB	ALA	608	57.070	-2.649	26.550	1.00	26.70
MOTA	4641	С	ALA	608	59.457	-1.850	26.368	1.00	25.97
ATOM	4642	0	ALA	608	59.802	-0.993	27.183	1.00	25.88
ATOM	4643	N	ARG	609	60.250	-2.848	25.994	1.00	26.02
MOTA	4645	CA	ARG	609	61.606	-2.977	26.512	1.00	30.44
ATOM	4646	CB	ARG	609	62.234	-4.285	26.058	1.00	34.09
ATOM	4647	CG	ARG	609	61.642	-5.516	26.682	1.00	39.24
ATOM	4648	CD	ARG	609	62.659	-6.615	26.615	1.00	42.75
ATOM	4649	NE	ARG	609	63.405	-6.704	27.860	1.00	45.52
ATOM	4651	CZ	ARG	609	64.525	-7.405	28.019	1.00	46.24
ATOM	4652	NH1	ARG	609	65.055	-8.079	27.001	1.00	41.48
ATOM	4655	NH2	ARG	609	65.079	-7.482	29.225	1.00	47.49
ATOM ATOM	4658	c o	ARG ARG	609	62.478	-1.829	26.015	1.00	34.20
ATOM	4659 4660			609 610	63.265	-1.255	26.788	1.00	35.24
ATOM	4662	N CA	GLY GLY	610	62.368 63.130	-1.528 -0.439	24.717 24.138	1.00	33.25 29.57
ATOM	4663	C	GLY	610	62.802	0.814	24.138	1.00	29.37
ATOM	4664	0	GLY	610	63.695	1.543	25.335	1.00	27.46
ATOM	4665	И	MET	611	61.507	1.020	25.147	1.00	31.07
ATOM	4667	CA	MET	611	61.016	2.178	25.889	1.00	30.09
ATOM	4668	CB	MET	611	59.493	2.280	25.782	1.00	29.51
ATOM	4669	CG	MET	611	58.997	2.655	24.404	1.00	28.21
ATOM	4670	SD	MET	611	59.760	4.175	23.787	1.00	29.00
ATOM	4671	CE	MET	611	59.350	5.335	25.039	1.00	25.91
ATOM	4672	C	MET	611	61.439	2.189	27.361	1.00	
ATOM	4673	0	MET	611	61.734	3.242	27.361	1.00	30.47 29.43
ATOM	4674	N	GLU	612	61.429	1.031	28.002	1.00	31.97
ATOM	4676	CA	GLU	612	61.836	0.947	29.402	1.00	35.34
ATOM	4677	CB	GLU	612	61.707	-0.490	29.904	1.00	36.17
ATOM	4678	CG	GLU	612	62.305	-0.729	31.278	1.00	34.87
ATOM	4679	CD	GLU	612	62.259	-2.185	31.705	1.00	32.68
ATOM	4680	OE1	GLU	612	62.641	-3.070	30.904	1.00	35.01
		~~~				5.070	JU. JUZ	<b></b> • •	JJ. UI

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	ATOM	4681	OE2	GLU	610							
	ATOM	4682	С	GLU	612	61.8		-2.	443 3	32.858	1 00	
	ATOM	4683	0	GLU	612	63.2				9.490	1.00	
	ATOM	4684	N	TYR	612	63.6				0.417	1.00	
	ATOM	4686	CA		613	64.0				8.491	1.00	31.21
		4687	CB	TYR	613	65.4				8.440	1.00	36.10
1		4688	CG	TYR	613	66.2				7.301	1.00	34.76
1		1689	CD1	TYR	613	67.7	00				1.00	31.15
7		1690		TYR	613	68.6	00	0.6		7.284	1.00	34.28
		691	CE1	TYR	613	69.9		1.0		3.207	1.00	36.50
		692	CD2	TYR	613	68.1		2.1		3.219	1.00	38.20
	<b>~</b> ~		~~	TYR	613	69.52	20	2.5		.366	1.00	32.99
				TYR	613	70.39		1.9		.372	1.00	33.32
				TYR	613	71.72				.302	1.00	36.59
				ľYR	613	65.58		2.3		.333	1.00	35.73
	2000			ľYR	613	66.23		2.9		.273	1.00	34.03
				EU	614	64.91	<u> </u>	3.64		.075	1.00	35.26
			CA I	ŒU	614	64.94	- -	3.50		.250	1.00	31.78
			CB L		614	64.09	-	4.93		998	1.00	29.50
					514	64.564		5.29			1.00	28.26
			D1 L		514			4.74			1.00	31.29
			D2 L		14	63.564	ł	5.08		20-		28.09
AT		05 C	L.	_	14	65.951		5.28	2 24,			29.52
AT		_			14	64.489		5.71	5 28.	_		
ATO		07 N			15	65.108		6.71	7 28.			32.49
ATO		09 C		-	15	63.431		5.23	28.			31.73
ATO		LO CE			15	62.906		5.870	30.0			33.06
ATC		11 C	AL	-	15	61.598		5.192	30.5			35.16
ATC		.2 0	AL	_	15	63.942		5.838	31.2			6.64
ATO			SE			64.065		6.805	31.9			5.36
ATO		5 CA		_	16	64.690	4	4.739	31.3		_	6.80
ATO:	M 471					65.716		1.621				5.91
ATO	M 471					66.287		1.199				5.78
ATO		_	SE			67.133		.899	31.3			2.52
ATO			SE			66.832		.623	32.0			9.64
ATON	472					67.556		.048	32.96			7.48
ATOM			LYS			66.971		.980	30.79			3.76
ATOM	1 4724		LYS			67.973		. 931	30.35			. 74
ATOM	4725		LYS			68.540		.520	28.99			.44
ATOM			LYS			69.330		.232	29.04			. 94
ATOM	4727		LYS	617		70.539		402	29.93			.64
ATOM			LYS	617		71.252		091	30.13			.45
ATOM			LYS	617	'	72.552		306				. 84
ATOM		C	LYS	617	' ·	67.376	8	325	30.81			.49
ATOM	4734	0	LYS	617	(	57.909	9	188	30.28			.29
ATOM	4736	N	LYS	618	6	6.245	a.	528	29.59			. 95
ATOM		CA	LYS	618	6	55.569		822	30.952		0 34	87
ATOM	4737	CB	LYS	618	6	6.512	10.		30.997	_		44
ATOM	4738	CG	LYS	618	6	7.192			31.581		0 40.	
ATOM	4739	CD	LYS	618	6	6.234	10.4	146	32.877		0 48.	
	4740	CE	LYS	618	6	6.962	10.3		34.037	-	0 55.	47
ATOM	4741	NZ	LYS	618	6	6.070	9.9	39	35.310	1.00		
MOTA	4745	С	LYS	618		5.015	10.0		36.514	1.00		
ATOM	4746	0	LYS	618		4.557	10.3		29.663	1.00		
ATOM	4747	N	CYS	619	ر ج	z.35/	11.4	63	29.569	1.00		
ATOM	4749	CA	CYS	619	O:	5.006	9.4	72	28.647	1.00		
			-		64	1.525	9.8		27.323	1.00		
33SD/55	145. v01									- 0	-4.0	· &



										31.1	7
			_	<b>610</b>	6	5.279	9.033	26.263	1.00		
MOTA	4750	CB	CYS	619		4.816	9.306	24.541	1.00		
MOTA	4751	SG	CYS	619	6	3.004	9.701	27.149	1.00		24
MOTA	4752	C	CYS	619	6	2.418	8.649	27.388	1.00		14
ATOM	4753	0	CYS	619	6	2.359	10.798	26.800	1.00		76
ATOM	4754	N	ILE	620	6	0.935	10.822	26.542	1.00		
MOTA	4756	CA	ILE	620		0.268	12.040	27.193	1.00		
MOTA	4757	CB	ILE	620		8.799	12.116	26.774	1.0		
MOTA	4758	CG2	ILE	620	-	50.392	11.957	28.712	1.0		
MOTA	4759	CG1	ILE	620		50.016	13.236	29.396	1.0		96
MOTA	4760	CD1	ILE	620		60.864	10.961	25.023	1.0		70
MOTA	4761	С	ILE	620		61.384	11.920	24.465	1.0		70
MOTA	4762	0	ILE	620		60.249	9.986	24.366	1.0		
MOTA	4763	N	HIS	621		60.133	9.973	22.906	1.0		.61
MOTA	4765	CA	HIS			59.708	8.578	22.430	1.0		.62
MOTA			HIS			59.903	8.344	20.96		_	.49
ATOM		CG	HIS			60.511	7.336	20.30			.08
ATOM		CD2				59.373	9.168	19.98			.00
ATOM		ND1				59.637	8.669	18.79			.55
MOTA						60.325	7.554	18.95			.51
MOTA						59.194	11.026	22.32		-	.79
MOTA			HI			59.466	11.57	0 21.25			5.26
ATO	477		HI			58.048	11.24	8 22.96			4.68
ATO	M 477		AR			57.068	12.23				3.43
OTA						57.705	13.62	8 22.37		-	1.52
OTA					22	58.285	14.13	5 23.6		· ·	7.82
ATO					22	58.781	15.56	3 23.5		•	8.82
ATO		1 CD		_	22	59.216	16.05	0 24.8			0.41
ATC		2 NE			22	60.362	15.71	5 25.4		•	1.15
ATC					22	61.215	14.89	91 24.8			30.83
OTA					22 22	60.640	16.10	58 26.6			34.71
TA			_			56.283	11.8	91 21.2			35.58
TA	OM 47				22 22	55.289	12.5	44 20.9			34.90
AT	OM 47		_		523	56.719	10.8	84 20.4			34.30
TA	OM 47		_	-	523	55.986	; 10.4	68 19.2			36.76
AT	OM 47	95 C	_		623	56.443	11.2				43.35
AT	OM 47		_		623	55.53	5 10.9				47.64
AT	OM 47	-			623	55.980	) 11.]			1.00	43.30
PA	OM 47		-		623	54.37	g 10.4			1.00	32.24
A.					623	56.09	4 8.5	967 19.		1.00	31.19
A <sup>r</sup>		300	-	ASP	623	56.40			-	1.00	32.27
A'			_	ASP	624	55.89	5 8.	_	118	1.00	33.18
A'	TOM 4			LEU	624	55.96	4 6.	759 20.	005		31.16
A	TOM 4		_	LEU	624	56.01	.3 6.		390	1.00	32.74
A	TOM 4	• • •		LEU	624	56.01	.9 4.		452		30.64
А	TOM 4	• • •	CG	LEU	624	57.25	57 4.		.765	1.00	34.51
A	TOM 4	• • •	CD1	LEU	624	55.9	74 4.	-	.904	1.00	35.18
P	TOM 4	808	CD2	LEU		54.7			.217	1.00	35.72
1	ATOM 4	1809	C	LEU	624 624	53.5	89 6		.612	1.00	32.37
		1810	0	LEU	625	54.9	97 5		.084	1.00	30.60
1		4811	N	ALA	625	53.9	46 5		.223	1.00	25.26
	MOTA	4813	CA	ALA		53.4	47 6		.298	1.00	29.87
	MOTA	4814	CB	ALA	625	54.6	18 4		.427	1.00	32.01
		4815	С	ALA	625 625			.978 16	3.378	1.00	J2.V1
	MOTA	4816	0	ALA	023						

							-	, 0					
	ATOM	4817	N	ALA	626	5.5							
	ATOM	4819	CA	ALA	626	53.	. 834		.163	15	.779	1.00	20.30
	ATOM ATOM	4820	CB	ALA	626	54. 52	373 231	2	.057		978	1.00	30.12 29.62
	ATOM	4821	C	ALA	626	55.	255 255		.159	14.	441	1.00	27.11
	ATOM	4822	0	ALA	626	56	193		. 552	13.	838	1.00	26.57
	ATOM	4823	N	ARG	627	54.	423 935		871		434	1.00	26.29
	_	4825 4826	CA		627	55.	706		730	13.		1.00	26.74
	N 0700 .	4827	CB		627	55.	056	4. E	352	12.		1.00	28.73
		4828	CG		527	54.8	394		671 659	11.		1.00	29.62
		4829	CD NE		527	54.4	135		032	12.9		1.00	31.84
		831	CZ		27	53.9	87		878	12.4		1.00	38.54
A		1832			27	52.7	45		_	13.5		1.00	38.59
A	ma	~			27	51.8	22			14.0		1.00	39.55
A'	ma		_		27	52.4	47	9.6		13.5		1.00	35.96
A.	TIO		_	_	27	57.1	51	4.6		15.1		1.00	41.05
A			'		27	58.05	85	4.6		12.6		1.00	30.79
A	00	0.4.0			8 2	57.34	17	4.8		11.8		00	30.16
AT			`	ASN 62		58.66	1	5.1		13.98		.00	30.31
AT				ASN 62		58.58	7	6.2		4.55		.00	28.50
	OM 48			SN 62		58.36	9	7.5		5.54	_	.00 2	27.84
AT	OM 48			SN 62 SN 62		58.89	3	7.79		4.86	_	.00 3	31.41
AT		49 C				57.55	1	8.42		3.78 5.46		.00 3	3.45
ATO				_		59.352	2	3.91		5.16			8.53
ATO						60.232		4.07		5 - 02			8.10
ATC		53 C	_	AL 629		58.887	7	2.73		1.803			8.64
ATC	M 489					59.484		1.48		.253			7.79
ATO						58.475		0.57		. 983			B.30
ATO		6 CG		-		59.118	- (	0.75	3 16	. 284	1. 1.	-	5.38
ATO		7 C	VA			57.980		1.246	5 17	.265	1.	-	3.07
ATO		_	VA			59.925		0.810	13	. 949	1.(		. 48
IOTA NOTA	_		LE			59.114	c	616	13	. 043	1.0		.69
ATON			LE			61.220 61.749	0	.542	13	. 823	1.0		.07
ATOM			LE			62.999		.081	12.	616	1.0		.54 .17
ATOM			LE			62.831		.659	12.	142	1.0	~ •	.62
ATOM						54.121		.180	12.	035	1.0		14
ATOM			LEU			51.693		. 795		579	1.0		83
ATOM			LEU	630	ε	2.036	2.	543	11.		1.0		59
ATOM		_	LEU		6	2.290		541	12.		1.00		50
ATOM	4870		VAL	631		1.966		910	14.		1.00	31.	
ATOM	4871	CA	VAL	631	6	2.174		376 813	11.8		1.00	33.	
ATOM	4872	CB	VAL	631	6	0.902	-4.	EUE 013	12.0	022	1.00	31.	
ATOM	4873	CG1	VAL	631	6	1.017	-6.	003 067	11.5	82	1.00	29.4	
ATOM	4874	CG2 C	VAL	631	5	9.644	-3.	00 / 00 /	11.9	80	1.00	29.3	
ATOM	4875	0	VAL	631	6:	3.379	-4.3	242	12.1	96	1.00	25.3	
ATOM	4876	Ŋ	VAL	631	63	3.508	-3.8	265	11.1		1.00	32.3	17
MOTA	4878	CA	THR	632	64	.285	-4.9	107	10.0		1.00	33.5	7
ATOM	4879	CB	THR	632	65	.504	-5.4	52	11.8		1.00	34.3	
ATOM	4880	OG1	THR	632	66	.659	-5.6	85	11.14		1.00	35.8	4
ATOM	4882	CG2	THR	632	66	.328	-6.7	74	12.14		1.00	33.1	1
ATOM	4883	C	THR	632	66	. 922	-4.4		13.02		1.00	34.8	8
ATOM	4884	0	THR	632	65	.272	-6.7		12.97 10.35		1.00	28.89	
ATOM	4885	N	THR GLU	632	64	.195	-7.3		10.35		1.00	37.63	3
			3TO	633	66	.289	-7.16	5 3	9.60		.00	37.20	
SSSD/551	145. v01							-	2.60	· 1	.00	39.78	1

MOTA	4887	CA	GLU	633	66.182	-8.379	8.794	1.00	43.30
MOTA	4888	CB	GLU	633	67.437	-8.590	7.933	1.00	46.66
MOTA	4889	CG	GLU	633	67.336	-9.729	6.876	1.00	51.37
ATOM	4890	CD	GLU	633	66.490	-9.404	5.622	1.00	54.30
ATOM	4891	OE1	GLU	633	65.859	-8.327	5.523	1.00	55.85
ATOM	4892	OE2	GLU	633	66.460	-10.256	4.710	1.00	55.95
MOTA	4893	C	GLU	633	65.919	-9.592	9.67 <b>7</b>	1.00	42.72
MOTA	4894	0	GLU	633	65.360	-10.582	9.222	1.00	45.10
ATOM	4895	N	ASP	634	66.287	-9.494	10.949	1.00	42.83
MOTA	4897	CA	ASP	634	66.075	-10.585	11.884	1.00	43.03
ATOM	4898	CB	ASP	634	67.324	-10.809	12.743	1.00	49.02
ATOM	4899	CG	ASP ·	634	68.539	-11.240	11.916	1.00	55.95
ATOM	4900	OD1	ASP	634	68.462	-12.292	11.237	1.00	59.10
ATOM	4901	OD2	ASP	634	69.568	-10.525	11.943	1.00	59.41
ATOM	4902	С	ASP	634	64.848	-10.340	12.751	1.00	41.75
MOTA	4903	0	ASP	634	64.737	-10.873	13.847	1.00	42.79
ATOM	4904	N	ASN	635	63.937	-9.508	12.257	1.00	42.51
MOTA	4906	CA	ASN	635	62.686	-9.186	12.939	1.00	42.53
MOTA	4907	CB	ASN	635	61.768	-10.417	12.992	1.00	45.07
MOTA	4908	CG	ASN	635	61.483	-10.985	11.624	1.00	46.54
MOTA	4909	OD1	ASN	635	60.868	-10.336	10.786	1.00	49.77
MOTA	4910	ND2	ASN	635	61.949	-12.192	11.383	1.00	49.29
MOTA	4913	С	ASN	635	62.801	-8.577	14.331	1.00	40.51
ATOM	4914	0	ASN	635	61.939	-8.800	15.187	1.00	41.80
ATOM	4915	N	VAL	636	63.844	-7.795	14.561	1.00	37.98
ATOM	4917	CA	VAL	636	64.016	-7.164	15.856	1.00	33.92
ATOM	4918	CB	VAL	636	65.517	-7.005	16.195	1.00	32.21
ATOM	4919	CG1	VAL	636	65.697	-6.284	17.530	1.00	31.40
ATOM	4920	CG2	VAL	636	66.169	-8.367	16.242	1.00	30.93
ATOM	4921	C	VAL	636	63.349	-5.797	15.811	1.00	31.85
ATOM	4922	0	VAL	636	63.531	-5.061	14.849	1.00	33.47
ATOM	4923	N	MET	637	62.525	-5.492	16.807	1.00	31.69
ATOM	4925	CA	MET	637	61.860	-4.194	16.879	1.00	31.44
ATOM	4926	CB	MET	637	60.642	-4.241	17.820	1.00	34.97
ATOM ATOM	4927 4928	CG	MET	637	59.559	-5.264	17.455	1.00	36.80
ATOM	4928	SD CE	MET MET	637 637	58.860	-5.048	15.803	1.00	35.45
ATOM	4930	CE	MET	637	59.030 62.874	-6.709 -3.209	15.116	1.00	32.12
MOTA	4931	0	MET	637	63.512	-3.209	17.454 18.479	1.00	31.86
ATOM	4932	N	LYS	638	62.985			1.00	29.47
ATOM	4934	CA	LYS	638	63.915	-2.041 -0.994	16.820 17.244	1.00	30.87
ATOM	4935	CB	LYS	638	65.161				29.66
ATOM	4936	CG	LYS	638	66.171	-0.983 -2.059	16.349 16.691	1.00	27.51
ATOM	4937	CD	LYS	638	67.370		15.781	1.00	27.29
ATOM	4938	CE	LYS	638	68.409	-1.984 -3.029	16.150	1.00	28.55
ATOM	4939	NZ	LYS	638	68.964			1.00	24.75
ATOM	4943	C	LYS	638		-2.785	17.498	1.00	25.59
ATOM	4944	0	LYS	638	63.283 62.918	0.383 0.869	17.215 16.146	1.00 1.00	27.72
ATOM	4945	N	ILE	639	63.163				27.66
ATOM	4947	CA	ILE	639	62.597	1.004 2.343	18.387 18.501	1.00	26.21 26.27
ATOM	4948	CB	ILE	639	62.580	2.862	19.965	1.00	
ATOM	4949	CG2	ILE	639	61.896	4.206	20.017	1.00	26.52
ATOM	4950	CG1	ILE	639	61.898	1.854	20.017	1.00	21.50
ATOM	4951	CD1	ILE	639	60.496	1.654	20.526	1.00	25.70 25.62
					00.490	エ・セフセ	とし、コフフ	1.00	43.04

ATOM 4952 C ILE 639 63.505 1.288 17.718 1.00 29.56 ATOM 4954 N ALA 640 62.897 4.101 16.857 1.00 27.74 ATOM 4956 N ALA 640 62.897 4.101 16.057 1.00 27.74 ATOM 4957 CB ALA 640 63.620 5.071 16.042 1.00 28.75 ATOM 4958 C ALA 640 63.620 5.071 16.042 1.00 28.77 ATOM 4958 C ALA 640 63.620 5.071 16.042 1.00 28.77 ATOM 4958 C ALA 640 63.620 7.071 16.042 1.00 28.91 ATOM 4959 O ALA 640 63.620 7.74 4.796 14.563 1.00 28.91 ATOM 4959 C ALA 640 63.620 7.74 4.796 14.563 1.00 28.91 ATOM 4959 C ALA 640 63.620 7.74 4.796 14.563 1.00 28.91 ATOM 4959 C ALA 640 63.620 7.74 4.796 14.563 1.00 28.91 ATOM 4950 N ASP 641 63.007 7.464 16.067 1.00 28.25 ATOM 4964 CG ASP 641 62.960 9.393 15.248 1.00 33.44 ATOM 4965 OL ASP 641 62.869 9.393 15.948 1.00 33.44 ATOM 4965 OL ASP 641 62.869 9.393 15.948 1.00 33.44 ATOM 4966 N ASP 641 63.501 9.847 13.160 1.00 42.41 ATOM 4966 N ASP 641 63.501 9.847 13.160 1.00 42.41 ATOM 4969 N ASP 641 63.501 9.847 13.160 1.00 42.41 ATOM 4969 N ASP 641 63.501 9.847 13.160 1.00 42.97 ATOM 4969 N ASP 641 63.501 9.847 13.160 1.00 42.97 ATOM 4969 N ASP 641 63.501 9.847 10.309 18.020 1.00 28.42 ATOM 4971 CD PHE 642 64.138 8.604 18.663 1.00 29.67 ATOM 4973 CD PHE 642 64.347 7.656 20.890 1.00 28.42 ATOM 4973 CD PHE 642 66.368 7.559 21.219 1.00 23.96 ATOM 4974 CDI PHE 642 66.988 7.559 21.219 1.00 23.96 ATOM 4975 CD PHE 642 65.702 7.058 20.890 1.00 23.96 ATOM 4978 CZ PHE 642 66.984 5.590 19.501 1.00 23.20 ATOM 4978 CZ PHE 642 66.984 5.590 19.501 10.00 23.20 ATOM 4980 N PHE 642 66.888 7.559 21.219 1.00 23.96 ATOM 4978 CZ PHE 642 66.984 5.590 19.501 10.00 23.20 ATOM 4980 N PHE 642 66.984 7.559 21.219 1.00 23.90 ATOM 4980 N PHE 642 66.884 7.559 21.219 1.00 23.90 ATOM 4980 N PHE 642 66.884 7.559 21.219 1.00 23.90 ATOM 4980 N PHE 642 66.884 7.559 21.219 1.00 23.90 ATOM 4980 N PHE 642 66.570 19.580 19.591 1.00 23.20 ATOM 4980 N PHE 642 66.584 7.559 21.219 1.00 23.20 ATOM 4980 N PHE 642 66.580 1.00 28.91 19.576 1.00 23.20 ATOM 4980 N PHE 642 66.580 1.00 28.91 19.576 1.00 23.20 ATOM 4980 N PHE 642 66.580 1.00 28.91 19.576 1.00 23.20								T.8	0				
ATOM 4953 O ILE 639 64.730 3.288 17.7.18 1.00 29.56 ATOM 4956 CA ALA 640 62.897 4.101 16.857 1.00 27.91 ATOM 4956 CA ALA 640 63.377 4.796 14.553 1.00 28.79 ATOM 4959 C ALA 640 63.377 4.796 14.553 1.00 28.79 ATOM 4959 O ALA 640 63.377 4.796 14.553 1.00 28.79 ATOM 4960 N ASP 641 62.087 6.633 16.956 1.00 28.67 ATOM 4962 CA ASP 641 62.087 6.633 16.956 1.00 28.67 ATOM 4962 CA ASP 641 62.520 9.319 15.428 1.00 38.07 ATOM 4964 CG ASP 641 62.520 9.319 15.428 1.00 38.01 ATOM 4965 ODI ASP 641 62.080 9.393 13.948 1.00 38.01 ATOM 4966 OD ASP 641 62.080 9.807 13.100 42.41 ATOM 4966 OD ASP 641 62.869 9.319 15.428 1.00 38.01 ATOM 4968 O ASP 641 62.807 1.00 13.574 1.00 42.41 ATOM 4968 O ASP 641 62.807 9.393 13.948 1.00 38.01 ATOM 4968 O ASP 641 62.807 9.807 13.100 10.00 42.41 ATOM 4968 O ASP 641 62.807 9.807 13.100 10.00 42.41 ATOM 4969 N PHE 642 64.036 8.807 18.608 18.00 1.00 29.07 ATOM 4971 CD PHE 642 64.036 8.001 18.603 1.00 29.69 ATOM 4972 CB PHE 642 64.036 8.001 18.603 1.00 29.69 ATOM 4973 CD PHE 642 66.808 7.559 21.219 1.00 23.66 ATOM 4976 CE I PHE 642 66.808 7.559 20.980 1.00 23.06 ATOM 4976 CE I PHE 642 66.809 6.992 20.980 1.00 23.06 ATOM 4976 CE I PHE 642 68.000 6.992 20.980 1.00 23.06 ATOM 4976 CE PHE 642 66.808 5.993 20.121 1.00 24.08 ATOM 4979 C PHE 642 66.009 5.093 20.121 1.00 24.08 ATOM 4979 C PHE 642 66.009 5.903 20.121 1.00 24.08 ATOM 4980 N CLEU 644 65.520 14.00 39.01 1.00 33.29 ATOM 4980 N CLEU 644 65.520 14.00 39.01 1.00 33.00 ATOM 4980 N CLEU 644 65.520 14.00 39.01 1.00 32.99 ATOM 4980 C CLEU 644 65.520 14.00 39.01 1.00 31.29 ATOM 4990 C C ALA 645 66.414 18.699 18.124 1.00 35.29 ATOM 4991 CD LEU 644 65.520 14.00 31.00 42.61 ATOM 4990 C C ALA 645 66.414 18.699 18.124 1.00 54.78 ATOM 4990 C C ALA 645 65.585 16.601 18.080 1.00 55.41 ATOM 4990 C C ALA 645 65.585 16.601 18.080 1.00 55.41 ATOM 4990 C C ALA 645 65.595 11.00 12.00 55.41 ATOM 5000 O ALA 645 66.414 18.699 18.124 1.00 55.41 ATOM 5000 O ALA 645 65.595 11.00 11.00 55.41 ATOM 5000 O ALA 645 66.414 18.699 18.124 1.00 55.41 ATOM 5000 O ALA 645 66.414 18.699		ATOM	4952	C	TIE	624							
ATOM 4954 N ALA 640 63.620 5.071 16.00 29.566 ATOM 4955 CA ALA 640 63.620 5.071 16.032 1.00 27.74 ATOM 4958 C ALA 640 63.620 5.071 16.042 1.00 22.791 ATOM 4958 C ALA 640 63.377 4.796 14.563 1.00 28.79 ATOM 4950 N ALA 640 63.164 6.487 16.385 1.00 28.79 ATOM 4960 N ASP 641 64.007 7.464 16.067 1.00 28.25 ATOM 4963 CB ASP 641 63.708 8.876 16.296 1.00 28.25 ATOM 4963 CB ASP 641 62.869 9.319 15.428 1.00 33.44 ATOM 4965 OD1 ASP 641 62.869 9.319 15.428 1.00 33.44 ATOM 4965 OD1 ASP 641 62.869 9.393 13.948 1.00 38.01 ATOM 4966 OD2 ASP 641 62.006 9.847 13.160 1.00 42.41 ATOM 4966 OD2 ASP 641 63.501 9.311 17.745 1.00 42.71 ATOM 4968 O ASP 641 63.501 9.311 17.745 1.00 42.71 ATOM 4969 N PHE 642 64.138 8.604 18.663 1.00 28.42 ATOM 4971 CC PHE 642 64.138 8.604 18.663 1.00 29.62 ATOM 4972 CB PHE 642 64.130 8.604 18.663 1.00 29.62 ATOM 4973 CD PHE 642 64.347 7.656 20.693 1.00 27.18 ATOM 4974 CD1 PHE 642 66.888 7.559 21.219 1.00 23.66 ATOM 4975 CD2 PHE 642 66.888 7.559 21.219 1.00 23.66 ATOM 4979 C PHE 642 66.980 5.974 19.742 1.00 23.66 ATOM 4979 C PHE 642 66.980 5.974 19.742 1.00 23.66 ATOM 4979 C PHE 642 66.988 7.559 21.219 1.00 23.06 ATOM 4980 N PHE 642 66.980 5.990 20.121 1.00 23.02 ATOM 4980 C PHE 642 66.980 7.058 20.603 1.00 23.02 ATOM 4980 C PHE 642 66.980 1.035 2.70 ATOM 4980 C PHE 642 66.980 1.035 2.70 ATOM 4980 C PHE 642 66.980 1.035 2.70 ATOM 4980 C PHE 642 66.990 5.903 1.95 01 1.00 23.02 ATOM 4980 C PHE 642 66.990 5.903 1.95 01 1.00 23.02 ATOM 4980 C PHE 642 66.991 1.463 20.003 1.00 23.02 ATOM 4980 C PHE 642 66.991 1.463 20.003 1.00 23.02 ATOM 4980 C PHE 642 66.991 1.463 20.003 1.00 23.02 ATOM 4980 C PHE 642 65.502 14.603 19.501 1.00 23.02 ATOM 4980 C PHE 642 65.037 15.298 18.576 1.00 49.59 ATOM 4980 C PHE 642 65.037 15.298 18.576 1.00 49.59 ATOM 4990 C PHE 642 65.037 15.298 18.576 1.00 49.59 ATOM 4990 C PHE 644 65.502 14.603 19.607 1.00 55.44 ATOM 4990 C PHE 644 65.503 13.068 14.940 1.00 75.56 ATOM 5000 C ASP 652 50.389 652 50.389 22.241 11.600 75.68		ATOM						505	3	. 288 1	7 7		
ATOM 4956 CA ALA 640 62.897 4.101 16.857 1.00 27.79. ATOM 4957 CB ALA 640 63.377 4.796 14.553 1.00 28.97 ATOM 4959 C ALA 640 63.377 4.796 14.553 1.00 28.97 ATOM 4959 O ALA 640 63.376 4.796 14.553 1.00 28.97 ATOM 4960 N ASP 641 62.087 6.683 16.956 1.00 28.91 ATOM 4962 CA ASP 641 62.087 6.683 16.956 1.00 28.67 ATOM 4962 CA ASP 641 62.520 9.319 15.428 1.00 38.01 ATOM 4964 CG ASP 641 62.520 9.319 15.428 1.00 38.01 ATOM 4965 ODI ASP 641 62.080 9.393 13.948 1.00 38.01 ATOM 4966 OD ASP 641 62.080 9.393 13.948 1.00 38.01 ATOM 4966 OD ASP 641 62.080 9.847 13.160 1.00 42.41 ATOM 4968 O ASP 641 62.869 9.311 17.745 1.00 29.07 ATOM 4968 O ASP 641 62.847 10.309 18.020 1.00 29.07 ATOM 4970 CD PHE 642 64.347 8.914 20.074 1.00 29.69 ATOM 4971 CD PHE 642 64.361 8.914 20.074 1.00 29.69 ATOM 4972 CB PHE 642 66.848 7.559 21.219 1.00 23.96 ATOM 4973 CD PHE 642 65.828 5.974 19.742 1.00 23.96 ATOM 4974 CDI PHE 642 65.828 5.974 19.742 1.00 23.96 ATOM 4976 CE PHE 642 66.848 7.559 21.219 1.00 23.66 ATOM 4976 CE PHE 642 66.848 5.909 20.121 1.00 23.02 ATOM 4976 CE PHE 642 66.848 5.909 20.121 1.00 23.02 ATOM 4976 CE PHE 642 66.848 5.909 20.121 1.00 23.66 ATOM 4977 CE PHE 642 68.000 5.909 20.121 1.00 23.66 ATOM 4978 C PHE 642 66.949 5.909 20.121 1.00 23.66 ATOM 4978 C PHE 642 66.849 5.909 20.121 1.00 23.02 ATOM 4980 N DILY 643 66.699 11.463 20.003 1.00 32.99 ATOM 4981 N GLY 643 66.699 11.463 20.003 1.00 32.99 ATOM 4982 C LEU 644 65.520 14.043 17.745 1.00 32.10 ATOM 4988 C LEU 644 65.520 14.043 17.745 1.00 32.10 ATOM 4998 C LEU 644 65.520 14.043 17.745 1.00 32.10 ATOM 4998 C LEU 644 65.520 14.043 17.745 1.00 32.10 ATOM 4998 C LEU 644 65.520 14.03 19.501 1.00 32.99 ATOM 4998 C LEU 644 65.520 14.043 17.745 1.00 32.10 ATOM 4999 C ALEU 644 65.520 14.043 17.745 1.00 32.10 ATOM 4999 C ALEU 644 65.520 14.040 17.00 32.10 ATOM 4999 C ALEU 644 65.520 14.040 17.00 32.10 ATOM 4999 C ALEU 644 65.520 14.040 17.00 32.10 ATOM 4990 C ALEU 644 65.520 14.040 17.00 54.71 ATOM 4990 C ALEU 644 65.520 14.040 17.00 54.71 ATOM 4990 C ALEU 644 65.520 14.040 17.00 55.4		ATOM				639	64.	730					29.56
ATOM 4957 CB ALA 640 63.620 5.071 16.042 1.00 27.91 ATOM 4958 C ALA 640 63.154 4.796 14.563 1.00 26.74 ATOM 4959 O ALA 640 62.087 6.683 16.956 1.00 28.91 ATOM 4960 N ASP 641 64.007 7.464 16.067 1.00 28.25 ATOM 4963 CB ASP 641 63.708 8.876 16.296 1.00 38.67 ATOM 4963 CB ASP 641 62.869 9.319 15.428 1.00 33.44 ATOM 4963 CB ASP 641 62.869 9.319 15.428 1.00 33.44 ATOM 4965 OD1 ASP 641 62.869 9.319 13.948 1.00 33.44 ATOM 4965 OD2 ASP 641 62.869 9.393 13.948 1.00 38.01 ATOM 4966 OD2 ASP 641 62.869 9.011 31.574 1.00 42.41 ATOM 4967 C ASP 641 62.869 9.011 31.574 1.00 42.41 ATOM 4968 O ASP 641 62.869 9.011 31.574 1.00 42.41 ATOM 4967 N PHE 642 64.138 8.604 18.663 1.00 29.07 ATOM 4971 CD PHE 642 64.036 8.914 20.074 1.00 29.62 ATOM 4973 CG PHE 642 64.036 8.914 20.074 1.00 29.62 ATOM 4975 CD PHE 642 65.702 7.058 20.603 1.00 23.66 ATOM 4975 CD PHE 642 65.702 7.058 20.603 1.00 23.66 ATOM 4976 CE PHE 642 66.888 7.559 21.219 1.00 23.66 ATOM 4977 CE PHE 642 66.888 7.559 21.219 1.00 23.66 ATOM 4978 CZ PHE 642 66.89 5.974 19.742 1.00 24.08 ATOM 4980 O PHE 642 66.090 5.909 20.121 1.00 23.62 ATOM 4980 O PHE 642 66.090 5.909 20.121 1.00 23.62 ATOM 4981 N GLY 643 66.639 11.463 19.501 1.00 23.02 ATOM 4988 CA LEU 644 65.520 12.850 11.00 32.99 ATOM 4988 CA LEU 644 65.520 12.850 11.00 32.02 ATOM 4989 C PHE 642 64.755 10.664 12.574 10.0 32.09 ATOM 4981 C LEU 644 65.520 12.850 11.00 32.99 ATOM 4998 C LEU 644 65.520 12.850 11.00 32.99 ATOM 4998 C LEU 644 65.520 12.850 11.00 32.00 ATOM 4999 C PHE 642 64.755 10.664 13.666 19.333 1.00 35.29 ATOM 4999 C PHE 642 64.755 10.664 13.666 19.335 10.00 42.61 ATOM 4999 C PHE 642 64.755 10.664 13.666 19.335 10.00 42.61 ATOM 4998 C PHE 642 64.755 10.664 13.666 19.335 10.00 42.61 ATOM 4999 C PHE 642 64.755 10.664 13.666 19.335 10.00 42.61 ATOM 4999 C PHE 642 64.755 10.664 13.666 19.335 10.00 42.61 ATOM 4999 C PHE 642 65.702 12.850 18.592 10.00 42.61 ATOM 4999 C PHE 644 65.525 12.850 18.592 10.00 42.61 ATOM 4999 C PHE 644 65.525 12.850 18.859 10.00 42.61 ATOM 4999 C PHE 644 65.525 12.850 18.859 10.00 42.61 A							62.	897				1.00	
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ATOM 4964 CG ASP 641 62.520 9.319 15.428 1.00 33.80  ATOM 4965 OD1 ASP 641 62.869 9.393 13.948 1.00 38.01  ATOM 4966 OD2 ASP 641 62.006 9.847 13.150 1.00 42.41  ATOM 4967 C ASP 641 62.006 9.847 13.150 1.00 42.41  ATOM 4968 O ASP 641 62.847 10.309 18.020 1.00 29.07  ATOM 4971 CA PHE 642 64.138 8.604 18.663 1.00 29.69  ATOM 4972 CB PHE 642 64.036 8.914 20.074 1.00 29.69  ATOM 4973 CG PHE 642 66.036 8.914 20.074 1.00 29.69  ATOM 4973 CCD PHE 642 66.847 7.656 20.809 1.00 27.18  ATOM 4975 CE1 PHE 642 66.848 7.559 21.219 1.00 23.96  ATOM 4976 CE1 PHE 642 66.888 5.974 19.742 1.00 23.96  ATOM 4977 CE2 PHE 642 66.889 5.974 19.742 1.00 23.06  ATOM 4978 CZ PHE 642 68.090 5.909 20.121 1.00 23.02  ATOM 4979 C PHE 642 64.948 10.075 20.502 1.00 32.02  ATOM 4980 O PHE 642 64.755 10.664 21.574 1.00 32.10  ATOM 4981 N GLY 643 65.940 10.396 19.671 1.00 32.02  ATOM 4983 CA GLY 643 66.639 12.755 19.250 1.00 32.99  ATOM 4984 C GLY 643 66.869 11.463 20.003 1.00 32.99  ATOM 4986 N LEU 644 65.520 12.850 18.532 1.00 32.99  ATOM 4988 CA LEU 644 65.520 12.850 18.532 1.00 42.26  ATOM 4989 CB LEU 644 65.520 12.850 18.532 1.00 42.26  ATOM 4990 C G LEU 644 63.931 12.839 15.763 1.00 42.61  ATOM 4991 CD LEU 644 65.520 14.043 17.745 1.00 42.61  ATOM 4999 C LEU 644 63.931 12.839 15.763 1.00 45.59  ATOM 4999 C LEU 644 63.931 12.839 15.763 1.00 46.25  ATOM 4999 C LEU 644 63.931 12.839 15.763 1.00 46.25  ATOM 4999 C LEU 644 63.931 12.839 15.763 1.00 46.25  ATOM 4999 C LEU 644 65.037 15.298 18.578 1.00 45.65  ATOM 4999 C ALAA 645 65.491 13.849 18.90 1.00 52.08  ATOM 4999 C ALA 645 65.495 17.677 18.777 1.00 54.38  ATOM 4999 C ALA 645 65.495 17.677 18.777 1.00 54.38  ATOM 5000 O ALA 645 65.495 17.677 18.777 1.00 54.71  ATOM 5000 O ALA 645 65.495 17.677 18.777 1.00 54.71  ATOM 5000 O ALA 645 65.495 17.677 18.777 1.00 54.71  ATOM 5000 O ALA 645 65.495 17.677 18.777 1.00 54.71  ATOM 5000 O ALA 645 65.495 17.677 18.777 1.00 73.72  ATOM 5000 O ALA 645 65.495 17.677 18.777 1.00 73.72  ATOM 5000 O ALA 645 65.497 21.995 12.472 1.00 73.72  ATOM 5000 O ALA 645 6	1	3000					63.7	'08					28.25
ATOM 4966 OD1 ASP 641 62.869 9.393 13.948 1.00 38.01  ATOM 4966 OD2 ASP 641 62.006 9.001 13.574 1.00 42.41  ATOM 4968 O ASP 641 62.006 9.847 13.160 1.00 42.41  ATOM 4968 O ASP 641 63.501 9.311 17.745 1.00 29.07  ATOM 4969 N PHE 642 64.138 8.604 18.663 1.00 29.69  ATOM 4971 CA PHE 642 64.036 8.914 20.074 1.00 29.69  ATOM 4972 CB PHE 642 64.036 8.914 20.074 1.00 29.69  ATOM 4973 CG PHE 642 66.347 7.656 20.890 1.00 27.18  ATOM 4974 CD1 PHE 642 66.848 7.559 21.219 1.00 23.66  ATOM 4975 CD2 PHE 642 65.828 5.974 19.742 1.00 23.66  ATOM 4976 CZ PHE 642 68.200 6.992 20.980 1.00 23.02  ATOM 4978 CZ PHE 642 64.948 10.075 20.502 1.00 23.02  ATOM 4981 N GLY 643 66.869 11.463 20.003 10.00 23.20  ATOM 4983 CA GLY 643 66.869 11.463 20.003 10.00 23.20  ATOM 4983 CA GLY 643 66.869 11.463 20.003 10.00 23.20  ATOM 4985 N LEU 644 65.202 1.009 13.21 1.00 32.10  ATOM 4989 C GLY 643 66.391 1.275 10.00 32.99  ATOM 4989 C GLY 643 66.391 1.463 20.003 1.00 32.10  ATOM 4989 C GLY 643 66.391 1.463 20.003 1.00 32.10  ATOM 4989 C GLY 643 66.869 11.463 20.003 1.00 35.29  ATOM 4989 C GLY 643 66.391 1.263 10.00 35.29  ATOM 4989 C GLY 643 66.391 1.263 10.00 39.13  ATOM 4989 C GLEU 644 65.202 1.2850 18.532 1.00 42.266  ATOM 4989 C GLEU 644 65.202 12.850 18.532 1.00 42.266  ATOM 4999 C C LEU 644 65.202 12.850 18.532 1.00 42.266  ATOM 4999 C C LEU 644 65.203 13.068 14.940 1.00 45.65  ATOM 4999 C C LEU 644 65.391 15.298 18.574 1.00 45.65  ATOM 4999 C ALEU 644 65.191 13.016 14.889 1.00 45.65  ATOM 4999 C ALEU 644 65.591 15.298 18.570 1.00 45.55  ATOM 4999 C ALAA 645 65.585 16.401 18.080 1.00 55.44  ATOM 4999 C ALEU 644 65.591 15.298 18.570 1.00 73.83  ATOM 5000 C ALAA 645 66.595 17.607 18.777 1.00 55.471  ATOM 5000 C ALAA 645 65.595 16.601 11.989 1.00 73.83  ATOM 5000 C ALAA 645 65.595 17.607 18.777 1.00 55.44  ATOM 5000 C ALAA 645 65.595 17.607 18.779 1.00 73.79  ATOM 5000 C ALAA 645 65.595 17.607 18.799 1.00 73.79  ATOM 5000 C ALAA 645 65.595 17.607 18.799 1.00 73.79  ATOM 5000 C ALAA 655 65.595 17.607 18.799 1.00 73.79  ATOM 5000 C ALAA 645 65.595		N					62.5	20		_		1.00	
ATOM 4966 OD2 ASP 641 64.002 9.001 13.574 1.00 38.01  ATOM 4967 C ASP 641 62.006 9.847 13.160 1.00 42.41  ATOM 4968 O ASP 641 63.501 9.311 17.745 1.00 29.07  ATOM 4970 CA PHE 642 64.138 8.604 18.620 1.00 29.07  ATOM 4971 CA PHE 642 64.036 8.914 20.074 1.00 29.69  ATOM 4973 CG PHE 642 64.036 8.914 20.074 1.00 29.69  ATOM 4974 CD1 PHE 642 66.848 7.559 21.219 1.00 23.96  ATOM 4976 CE1 PHE 642 65.702 7.058 20.603 1.00 23.96  ATOM 4977 CE2 PHE 642 65.828 5.974 19.742 1.00 23.06  ATOM 4978 CZ PHE 642 66.848 7.559 21.219 1.00 23.06  ATOM 4979 C PHE 642 66.848 10.075 20.980 1.00 23.02  ATOM 4978 CZ PHE 642 67.069 5.403 19.501 1.00 23.02  ATOM 4980 O PHE 642 64.958 10.075 20.502 1.00 23.09  ATOM 4981 N GLY 643 65.940 10.396 19.671 1.00 21.68  ATOM 4984 C GLY 643 66.689 11.463 20.003 1.00 23.104  ATOM 4986 N LEU 644 65.202 14.003 12.755 19.250 1.00 39.13  ATOM 4989 CB LEU 644 65.202 14.003 1.00 39.83  ATOM 4989 CB LEU 644 65.520 12.850 18.532 1.00 42.26  ATOM 4999 CD LEU 644 63.931 13.666 19.333 1.00 39.83  ATOM 4999 CD LEU 644 63.931 13.843 16.911 1.00 44.59  ATOM 4999 CD LEU 644 65.191 13.066 19.333 1.00 44.56  ATOM 4999 CD LEU 644 65.520 14.003 17.745 1.00 42.66  ATOM 4999 CD LEU 644 65.520 14.003 17.775 1.00 42.66  ATOM 4999 CB LEU 644 65.520 14.003 17.775 1.00 42.66  ATOM 4999 CB LEU 644 65.037 15.281 15.663 1.00 43.66  ATOM 4999 CB LEU 644 65.037 15.281 15.663 1.00 43.66  ATOM 4999 CB LEU 644 65.037 15.281 15.663 1.00 43.66  ATOM 4999 CB LEU 644 65.037 15.281 15.663 1.00 43.66  ATOM 4999 CB ALAA 645 65.495 17.677 18.777 1.00 55.44  ATOM 4999 CB ALAA 645 66.414 18.699 18.124 1.00 73.83  ATOM 5000 C ALAA 645 66.503 18.882 19.832 1.00 45.65  ATOM 5000 C ALAA 645 65.501 12.995 12.475 1.00 56.69  ATOM 5000 C ALAA 645 65.501 12.995 12.475 1.00 73.71  ATOM 5000 C ALAA 645 65.503 18.882 19.832 1.00 73.71  ATOM 5000 C ALAA 645 65.503 18.504 11.569 1.00 75.568  ATOM 5000 C ALAA 645 65.503 19.495 12.475 1.00 75.568					ASP	641	62. B	69	9.3			1.00	
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ATOM 4990 CG LEU 644 63.911 12.839 15.763 1.00 44.59  ATOM 4991 CD1 LEU 644 62.653 13.068 14.940 1.00 42.61  ATOM 4993 C LEU 644 65.119 13.016 14.889 1.00 45.65  ATOM 4994 O LEU 644 65.037 15.298 18.578 1.00 49.59  ATOM 4995 N ALA 645 65.585 16.401 18.080 1.00 51.90  ATOM 4997 CA ALA 645 65.495 17.677 18.777 1.00 54.71  ATOM 4999 C ALA 645 66.414 18.699 18.124 1.00 54.38  ATOM 5000 O ALA 645 63.534 18.582 19.832 1.00 56.69  ATOM 5001 N ASP 652 52.389 21.543 14.759 1.00 56.69  ATOM 5004 CB ASP 652 51.207 21.745 13.934 1.00 73.83  ATOM 5005 CG ASP 652 50.398 22.241 11.569 1.00 73.74  ATOM 5006 OD1 ASP 652 50.398 22.241 11.569 1.00 73.71  ATOM 5008 C ASP 652 50.497 21.956 10.357 1.00 73.71  ATOM 5009 O ASP 652 50.321 20.514 14.042 1.00 75.96  ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96  ATOM 5012 CA TYR 653 48.348 19.524 15.064 1.00 75.68			9 CB				65.202	14.	043	17.74			
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ATOM 5003 CA ASP 652 52.389 21.543 14.759 1.00 56.69  ATOM 5004 CB ASP 652 51.207 21.745 13.934 1.00 73.74  ATOM 5005 CG ASP 652 51.601 21.995 12.472 1.00 73.22  ATOM 5006 OD1 ASP 652 49.354 22.715 12.065 1.00 73.71  ATOM 5008 C ASP 652 50.497 21.956 10.357 1.00 73.02  ATOM 5009 O ASP 652 50.321 20.514 14.042 1.00 75.11  ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96  ATOM 5013 CB TYR 653 47.274 19.914 15.000	ATOM					6	3.534	18.5	R2	10.790	_		4
ATOM 5004 CB ASP 652 51.207 21.745 13.934 1.00 73.74  ATOM 5005 CG ASP 652 51.601 21.995 12.472 1.00 73.22  ATOM 5006 OD1 ASP 652 49.354 22.715 12.065 1.00 72.95  ATOM 5008 C ASP 652 50.497 21.956 10.357 1.00 73.02  ATOM 5009 O ASP 652 50.321 20.514 14.042 1.00 75.11  ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96  ATOM 5013 CB TYR 653 47.274 19.914 15.000	ATOM					5	2.389			19.832			9
ATOM 5005 CG ASP 652 51.601 21.995 12.472 1.00 73.83  ATOM 5006 OD1 ASP 652 49.354 22.241 11.569 1.00 72.95  ATOM 5007 OD2 ASP 652 50.497 21.956 10.357 1.00 73.71  ATOM 5008 C ASP 652 50.321 20.514 14.042 1.00 75.11  ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96  ATOM 5013 CB TYR 653 47.274 19.914 15.064 1.00 75.68						5	1.207	23.5	4.5		1.00		
ATOM 5006 OD1 ASP 652 50.398 22.241 11.569 1.00 73.22 ATOM 5006 OD1 ASP 652 49.354 22.715 12.065 1.00 72.95 ATOM 5008 C ASP 652 50.497 21.956 10.357 1.00 73.71 ATOM 5009 O ASP 652 50.321 20.514 14.042 1.00 75.11 ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96 ATOM 5013 CB TYR 653 47.274 19.914 15.000					652	5	1.601	21./					
ATOM 5006 OD1 ASP 652 49.354 22.715 12.065 1.00 72.95 ATOM 5007 OD2 ASP 652 50.497 21.956 10.357 1.00 73.71 ATOM 5009 O ASP 652 50.321 20.514 14.042 1.00 75.11 ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96 ATOM 5013 CB TYR 653 47.274 19.914 15.009				ASP		E 4	001	∠1.99	95	12.472		•	
ATOM 5007 OD2 ASP 652 50.497 21.956 10.357 1.00 73.71 ATOM 5008 C ASP 652 50.321 20.514 14.042 1.00 75.11 ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96 ATOM 5013 CB TYR 653 47.274 19.914 15 000			OD1			) ات د م	v. 398	22.24	11				
ATOM 5008 C ASP 652 50.321 20.514 14.042 1.00 73.71 ATOM 5009 O ASP 652 50.568 19.495 13.394 1.00 75.11 ATOM 5012 CA TYR 653 49.272 20.628 14.849 1.00 75.57 ATOM 5013 CB TYR 653 47.274 19.914 16.000			OD2			4:	7.354	22.71	.5				
ATOM 5009 O ASP 652 50.321 20.514 14.042 1.00 73.02 ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.96 ATOM 5013 CB TYR 653 48.348 19.524 15.064 1.00 75.68		5008				50	0.497	21.95		10 357			
ATOM 5010 N TYR 653 49.272 20.628 14.849 1.00 75.57 ATOM 5013 CB TYR 653 47.274 19.914 16.000						50	321	20.51				73.02	?
ATOM 5012 CA TYR 653 49.272 20.628 14.849 1.00 75.96 ATOM 5013 CB TYR 653 48.348 19.524 15.064 1.00 75.68	ATOM					50	.568	19.40		10 22		75.11	
ATOM 5013 CB TYR 653 48.348 19.524 15.064 1.00 75.57 47.274 19.914 15.069					653			20 60		3.394		75.96	
25 11R 653 47.274 19.914 15.064 1.00 75.68					653			10 50		14.849	1.00		
19.914 16.000		2013	CB	TYR	653	47		10 5			1.00		
202L/33145. v01	SSSDIE	1.45				-,	/	±9.91	4 1	6.088			
	2220133	145. v01										, 0.05	



										0 79.	<b>5</b> 5
					4	7.771	19.995	17.519	1.0	-	
ATOM	5014	CG	TYR	653	•s. ∧	6.983	20.567	18.518	1.0		
MOTA	5015	CD1	TYR	653	4	7.438	20.648	19.836	1.0		
MOTA	5016	CE1	TYR	653	4	9.032	19.503	17.874			70
ATOM	5017	CD2	TYR	653	4	9.496	19.578	19.183			70
ATOM	5018	CE2	TYR	653	4	9.490	20.152	20.160	1.0		
ATOM	5019	CZ	TYR	653	4	8.698	20.243	21.45		00 83.	
	5020	OH	TYR	653	4	19.165	19.038	13.78		00 75.	
MOTA	5022	C	TYR	653		17.685	17.897	13.71			. 97
MOTA	5022	0	TYR	653	4	47.232	19.885	12.76	7 1.		.85
MOTA		Ŋ	TYR	654		47.679		11.50	7 1.		. 32
MOTA	5024	CA	TYR	654		47.039	19.538	10.97		00 71	.97
MOTA	5026	CB	TYR	654		46.276	20.750	11.95		00 70	. 94
MOTA	5027	CG	TYR	654		45.259	21.276	13.18		00 71	.41
MOTA	5028	CD1	TYR	654		45.659	21.801	14.12		.00 73	.60
MOTA	5029		TYR			44.733	22.234	14.12			.81
MOTA		CE1	TYR			43.899	21.206	11.68			.81
MOTA			TYR			42.956	21.642	12.61			.84
MOTA						43.380	22.152	13.83			5.60
MOTA	5033		TYR			42.457	22.571	14.7			3.82
MOTA	5034		TYF			47.975	18.967				4.25
ATOM	5036		TYF			47.545	18.671				4.04
ATOM	5037		TYI			49.249	18.806	10.7			5.41
MOTA	1 5038		LY			50.195	18.256	9.8			8.45
MOTA	1 504	D CA	LY			51.626	18.680	10.1		-	3.01
OTA		1 CB	ΓĀ			52.647	18.198	9.1	-	_	7.72
ATO		2 CG	LY			54.062	18.589	9.5	-		1.45
ATO		3 CD	ΓĀ			55.076	17.81	3 8.7			
ATO			LY			56.489	18.13	39.(			4.17
ATO			LY			56.409		6 9.1			75.50
ATO			L)			50.075		2 10.			75.90
OTA		_	L)			50.245		3 8.	672		75.26
ATC			L	rs 650		49.750		о в.	533		74.97
ATC			L	rs 65		49.597		6 7.	323	_	75.40
			3 L	YS 65	6	48.723		-	519		76.87
)TA		•		YS 65	6	47.266			239	1.00	80.75
ATC			_	YS 65	6	46.489		-	483	1.00	83.60
ATO				YS 65	6	45.00			204	1.00 .	87.14
ATC				YS 65	6	44.23	_		414	1.00	74.58
TA		_		YS 65	66	50.93	-		.897	1.00	75.01
		-			56	51.90			.736	1.00	59.18
•••					60	49.13		-	.848	1.00	56.19
					60	48.10	6 10.7	-	.192	1.00	55.31
	_				60	47.40		<b>-</b>	.328	1.00	56.96
					60	46.28				1.00	53.02
	_	•••			61	48.05	59 10.1		.183	1.00	49.80
A.					61	47.45	93 10.0		.527	1.00	51.79
A'		•			61	47.9	44 8.		.229	1.00	50.59
A'		•	_		61	47.6	83 7.		.450	1.00	53.68
A		• • •	CG		661	47.8	22 6.	_	367		52.66
A			CD	•	661	47.7	14 5.		9.665	1.00	51.73
A	TOM 5	075	NE	-		47.9	28 3.		0.236	1.00	50.23
		5077	CZ		661	48.2		794 1	1.518	1.00	52.58
		5078	NH1		661	47.8		751	9.528	1.00	
		5081	NH2		661	47.9		.297 1	0.346	1.00	44.80
		5084	С		661			. 998	9.986	1.00	43.61
		5085	0	ARG	661	40.0					

							182						
	MOTA	5086	N	T Tarr									
	ATOM	5088	CA	LEU	662	47.	221	11.528					
	ATOM	5089		LEU	662	47.		12.654			1.00	40.7	4
	ATOM	5090	CB	LEU	662	46.			12.3	133	1.00	37.8	
	ATOM		CG	LEU	662	45.		13.415	12.6	71	1.00	36.1	
	ATOM	5091	CD1	LEU	662	44.(		L4.074	11.4	99	1.00	35.3	
		5092	CD2	LEU	662	46.5		4.278	11.8		1.00		
	ATOM	5093	C	LEU	662	46.2		5.383	11.1		1.00	31.09	
	ATOM	5094	0	LEU		48.1	.62 1	2.170	13.6			34.37	
	ATOM	5095	N		662	47.5	29 l	1.479	14.4		1.00	35.34	
	ATOM	5096	CD		663	49.4	41 - 1	2.518			1.00	33.06	
	ATOM	5097			663	50.3	_	3.113	13.84		1.00	36.39	
			CA	PRO	663	50.1			12.86		.00	37.57	
		5098	CB	PRO (	663	51.5		2.107	15.05		.00	36.39	
	* _	5099	CG		63	51.5		2.787	14.88		.00		
		5100	C		63	51.72	_	2.657	13.40	_	.00	36.98	
			^	`	63	49.47		.491	16.37			38.48	
		5102		-		49.69	<sup>9</sup> 11	.841	17.39		.00	35.47	
	ATOM 5	5104			64	48.64	6 13		16.36		.00	35.08	
	3 /2		~-		64	47.95	1 13		10.36		.00	34.28	
					64	47.03			17.583		.00	34.43	
	3.000				64	47.88			17.376			36.92	
				'AL 6	54	46.09			17.160	1.		37.55	
		108 (	v	AL 66	54	47.13		989	16.186			38.28	
		109 ტ	) v	AL 66		47.13		749	18.120				
		110 N	L	YS 66		46.908	12.	641 ]	19.318	1.		3.03	
			_	YS 66		46.803	11.		7.236			4.62	
	TOM 51	113 C	_			46.040	10.		7.614	1.0		2.47	
	TOM 51	.14 C				45.456	9.	_		1.(		0.71	
A		.15 C		- •		44.324	10.		6.370	1.0		9.59	
A'	T	16 C	_			43.927	10.	_	5.768	1.0	00 2	9.64	
	TOM 51				5	42.664			4.367	1.0	0 3	1.86	
	TOM 51	_		- • •	5	42.296	11.0		3.899	1.0	0 30	0.42	
		~ -	LY	S 665	5	46.801	10.7		2.486	1.0		5.50	
		•	LY	S 665	5	46.230	9.6		3.498	1.0		2.23	
			TR.			40.230	8.6	59 18	955	1.0			
	OM 512		TR			48.080	9.9	15 18	.748	1.00		. 04	
	OM 512	6 CB				48.886	9.0		.619	1.00		. 38	
AT		7 CG				50.204	8.6		.945			.32	
AT	OM 512					50.078	7.5		.006	1.00		.07	
AT						49.531	7.5			1.00		. 26	
ATO		_				49.630	6.25		.684	1.00		. 07	
ATO				- 0 0		48.982			.163	1.00	26.		
ATC						50.473	8.56		882	1.00	26.		
ATO			-	666		50.206	6.23		234	1.00	24.		
ATO				666	4	9.190	5.46	-·•	132	1.00	27.		
				666	4	29.190	5.92		874	1.00			
ATO		CH2	TRP	666	7	8.548	8.24	8 14.		1.00	27.		
ATO	,	' c	TRP		4	8.658	6.93	4 14.			30.	14	
ATO		0		666		9.203	9.80		^	1.00	26.		
ATO	M 5139	-	TRP	666	4	9.688	9.202			1.00	33.8	84	
ATO			MET	667	4	8.905	11.099	• •		00	32.8	32	
ATON			MET	667	4	9.180	17 00-	-		.00	35.7		
ATOM		CB	MET	667	4	9.150	11.960		069 1	.00	37.6		
		CG	MET	667	E /		13.423	21.6		.00			
ATOM		SD	MET	667	) C	0.487	13.975	21.2		.00	41.9	· 5	
ATOM	2243	CE	MET		50	384	15.728	20.9	<b>-</b> -		48.4		
ATOM	5146	c	MET	667	50	711	15.745	19.1		.00	55.3		
ATOM	5147	ō		667	48	.294	11.802			.00	49.2		
ATOM			MET	667	47	_	11.699	23.2		.00	38.9	8	
	~~*0	N	ALA	668	48			23.1		.00	39.1	В	
SSSD	55145. vo:	_					11.824	24.4	56 1.	00	38.72		
JJJU/3	22145. VN1	ī										-	





ATOM	5150	CA	ALA	668	48.231	11.728	25.727	1.00	37.82
MOTA	5151	CB	ALA	668	49.224	11.527	26.857	1.00	38.49
MOTA	5152	С	ALA	668	47.497	13.051	25.891	1.00	38.16
ATOM	5153	0	ALA	668	47.937	14.072	25.363	1.00	37.21
ATOM	5154	N	PRO	669	46.383	13.062	26.644	1.00	39.78
MOTA	5155	CD	PRO	669	45.785	11.931	27.367	1.00	40.08
MOTA	5156	CA	PRO	669	45.598	14.281	26.858	1.00	40.68
MOTA	5157	CB	PRO	669	44.474	13.806	27.782	1.00	42.15
MOTA	5158	CG	PRO	669	44.346	12.352	27.446	1.00	42.56
ATOM	5159	C	PRO	669	46.398	15.432	27.484	1.00	42.69
ATOM	5160	0	PRO	669	46.320	16.566	27.019	1.00	42.14
MOTA	5161	N	GLU	670	47.168	15.153	28.532	1.00	43.21
ATOM	5163	CA	GLU	670	47.956	16.211	29.160	1.00	44.62
MOTA	5164	CB	GLU	670	48.651	15.719	30.429	1.00	44.95
ATOM	5165	CG	GLU	670	49.824	14.782	30.197	1.00	45.54
ATOM	5166	CD	GLU	670	49.422	13.332	30.079	1.00	42.72
MOTA	5167	OE1	GLU	670	50.332	12.481	30.066	1.00	41.43
MOTA	5168	OE2	GLU	670	48.212	13.036	30.015	1.00	44.44
ATOM	5169	C	GLU	670	48.993	16.772	28.195	1.00	44.88
ATOM	5170	0	GLU	670	49.248	17.968	28.194	1.00	45.08
ATOM	5171	N	ALA	671	49.565	15.908	27.358	1.00	44.75
ATOM	5173	CA	ALA	671	50.573	16.323	26.392	1.00	45.92
ATOM	5174	CB	ALA	671	51.256	15.095	25.766	1.00	44.10
ATOM	5175	C	ALA	671	49.944	17.193	25.314	1.00	47.96
ATOM	5176	0	ALA	671	50.526	18.192	24.894	1.00	49.16
MOTA	5177	N	LEU	672	48.729	16.836	24.917	1.00	49.84
ATOM	5179	CA	LEU	672	47.989	17.554	23.881	1.00	50.74
ATOM	5180	CB	LEU	672	46.926	16.619	23.289	1.00	53.20
ATOM -	5181	CG	LEU	672	46.184	16.989	22.004	1.00	55.26
ATOM	5182	CD1	LEU	672	47.153	17.155	20.856	1.00	57.12
ATOM	5183	CD2	LEU	672	45.203	15.895	21.680	1.00	52.86
ATOM	5184	C	LEU	672	47.327	18.826	24.408	1.00	50.79
ATOM	5185	0	LEU	672	47.302	19.855	23.736	1.00	50.95
ATOM	5186	N	PHE	673	46.792	18.751	25.618	1.00	52.07
ATOM	5188	CA	PHE	673	46.111	19.884	26.226	1.00	54.39
ATOM	5189	CB	PHE	673	44.892	19.396	27.019	1.00	51.21
ATOM	5190	CG	PHE	673	43.871	18.656	26.186	1.00	48.49
ATOM	5191	CD1	PHE	673	43.304	17.473	26.646	1.00	47.79
ATOM	5192	CD2	PHE	673	43.470	19.149	24.949	1.00	49.04
ATOM	5193	CE1	PHE	673	42.349	16.789	25.888	1.00	47.90
ATOM	5194	CE2	PHE	673	42.511	18.473	24.182	1.00	49.71
ATOM	5195	CZ	PHE	673	41.952	17.288	24.655	1.00	46.86
ATOM	5196	C	PHE	673	47.007	20.741	27.123	1.00	58.25
ATOM	5197	0	PHE	673	47.000	21.971	27.034	1.00	60.52
ATOM	5198	N	ASP	674	47.784	20.094	27.983	1.00	59.63
ATOM	5200	CA	ASP	674	48.652	20.815	28.905	1.00	62.11
ATOM	5201	CB	ASP	674	48.568	20.196	30.307	1.00	63.81
ATOM	5202	CG	ASP	674	47.143	20.015	30.791	1.00	66.46
ATOM	5203	OD1	ASP	674	46.815	18.901	31.247	1.00	66.70
MOTA	5204	OD2	ASP	674	46.354	20.981	30.722	1.00	68.77
ATOM	5205	C	ASP	674	50.119	20.852	28.482	1.00	63.36
ATOM	5206	0	ASP	674	50.979	21.175	29.310	1.00	64.11
ATOM	5207	N	ARG	675	50.410	20.486	27.228	1.00	62.94
ATOM	5209	CA	ARG	675	51.789	20.456	26.706	1.00	60.75





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		5210	CB	ARG	675	50.00					
	MOTA	5211	CG	ARG	675	-2.2		874 26	.360	1.00	60.56
		5212	CD	ARG	675	,		560 25	.261	1.00	63.67
	TOM 5	5213	NE	ARG	675	51.98		970 24	. 964	1.00	66.99
A	TOM S	215	CZ	ARG	675	53.30	8 23.		.337	1.00	
A	TOM 5	216	NH1	ARG		54.06	3 25.		173	1.00	69.34
A'	TOM 5		NH2		675	53.63	7 26.		590	1.00	68.48
A'			_	ARG	675	55.25	4 24.		593		65.81
A:			_	ARG	675	52.75	19.		700	1.00	68.76
			_	ARG	675	53.933	20.5		766	1.00	58.06
				ILE	676	52.221	18.8			1.00	59.30
				ILE	676	52.992				1.00	55.62
				ILE	676	52.154				1.00	54.09
				LE	676	52.749	-			1.00	52.69
	<b></b>		G1 ]	ILE	676	52.049				1.00	49.38
AT			D1 1		676	51.306				1.00	53.15
AT		31 C	ı		676	52.306		03 32.ε	45	1.00	57.79
ATO		32 O		_	676	53.468	16.7			1.00	53.83
ATO		33 N			577	52.668	15.8	91 28.7		L.00	
ATO	DM 52	35 C.	_			54.773	16.67	71 28.7		00	54.87
ATO			_		577	55.343	15.43			00	51.76
ATC	DM 52:		_		77	56.232	15.72				49.42
ATO	M 523				77	55.466	16.18			.00	51.33
ATO	-				77	55.158	17.52				56.22
ATO		<b></b>		-	77	54.491	17.96				56.12
ATO					77	55.078	15.26			.00	56.18
ATO				R 6	77	54.411				.00	58.13
ATO		_ `		R 6	77	54.125	15.68			.00	57.65
		_	TY	R 6	77	53.504	17.03				8.23
ATO		_	TY	_	77	56.136	17.45				1.71
ATON	_		TY		77	56.983	14.73(				6.46
ATOM		7 N	TH				15.335		0 1.		8.65
ATOM		CA	TH			55.818	13.464				1.73
ATOM		CB	THI			56.498	12.664	30.53			9.83
ATOM	5253	L OG:				55.680	12.593	31.86			
ATOM	5253					54.462	11.867	31.642			1.78
ATOM			THE	- •		55.342	13.988	32.383			5.77
ATOM						56.661	11.242	30.011			L.84
ATOM			THR			56.258	10.917	28.897			7.46
ATOM	5258		HIS			57.264	10.388	30.825			7.51
ATOM	5259		HIS			57.423	9.003	30.457			.36
ATOM	5260	CB	HIS	679		58.348	8.294	31.439			. 91
ATOM	5261	CG	HIS	679	•	59.761	8.798		1.0		.05
ATOM		CD2	HIS	679	)	60.453	9.569	31.404	1.0		.68
ATOM	5262	ND1	HIS	679		60.632	8.507	32.278	1.0		.89
ATOM	5264	CE1	HIS	679		61.803		30.380	1.0	0 37	.49
	5265	NE2	HIS	679		61.721	9.071	30.621	1.0		. 58
ATOM	5267	C	HIS	679		56.032	9.722	31.766	1.0		.81
ATOM	5268	0	HIS	679		56.032 FE 772	8.376	30.441	1.0	_	. 76
ATOM	5269	N	GLN	680		55.771	7.458	29.660	1.00		
ATOM	5271	CA	GLN			55.126	8.908	31.264	1.00		
ATOM	5272	СВ	GLN	680		53.754	8.407	31.332	1.00		
ATOM	5273	CG		680		3.069	8.815	32.640			
ATOM	5274		GLN	680		3.645	8.128	33.884	1.00		
ATOM	5275	CD	GLN	680		3.676	6.595	33.780	1.00		
ATOM	5276	OE1	GLN	680	5	2.669	5.925		1.00		
ATOM		NE2	GLN	680		4.846	6.043	33.996	1.00		76
	5279	С	GLN	680		2.927	8.842	33.464	1.00	- •	57
SSSD/e-					_	- <del>- ·</del>	0.042	30.121	1.00		
SSSD/55	145. v01										



ATOM	5280	0	GLN	680	51.950	8.185	29.765	1.00	37.93
ATOM	5281	N	SER	681	53.282	9.961	29.504	1.00	36.38
ATOM	5283	CA	SER	681	52.563	10.367	28.306	1.00	38.05
ATOM	5284	CB	SER	681	52.857	11.819	27.940	1.00	41.41
ATOM	5285	OG	SER	681	54.239	12.069	27.938	1.00	42.92
MOTA	5287	C	SER	681	52.991	9.421	27.178	1.00	37.92
ATOM	5288	0	SER	681	52.205	9.148	26.263	1.00	37.21
ATOM	5289	N	ASP	682	54.237	8.932	27.248	1.00	34.77
MOTA	5291	CA	ASP	682	54.750	7.972	26.267	1.00	31.99
MOTA	5292	CB	ASP	682	56.243	7.683	26.481	1.00	31.08
ATOM	5293	CG	ASP	682	57.165	8.638	25.721	1.00	33.63
MOTA	5294	OD1	ASP	682	58.386	8.503	25.920	1.00	32.35
ATOM	5295	OD2	ASP	682	56.707	9.500	24.930	1.00	29.46
MOTA	5296	C	ASP	682	53.969	6.672	26.457	1.00	31.54
ATOM	5297	0	ASP	682	53.675	5.971	25.493	1.00	29.94
ATOM	5298	N	VAL	683	53.677	6.334	27.712	1.00	30.48
ATOM	5300	CA	VAL	683	52.913	5.126	28.023	1.00	32.94
MOTA	5301	CB	VAL	683	52.731	4.939	29.572	1.00	33.94
MOTA	5302	CG1	VAL	683	51.635	3.905	29.872	1.00	32.71
MOTA	5303	CG2	VAL	683	54.042	4.474	30.209	1.00	27.41
MOTA	5304	C	VAL	683	51.545	5.164	27.299	1.00	32.27
ATOM	5305	0	VAL	683	51.106	4.158	26.733	1.00	30.54
MOTA	5306	Ŋ	TRP	684	50.902	6.332	27.282	1.00	32.57
ATOM	5308	CA	TRP	684	49.616	6.477	26.600	1.00	32.76
ATOM	5309	CB	TRP	684	49.060	7.895	26.765	1.00	33.67
ATOM	5310	CG	TRP	684	47.855	8.210	25.891	1.00	38.22
ATOM	5311	CD2	TRP	684	46.503	8.435	26.328	1.00	39.96
ATOM	5312	CE2	TRP	684	45.734	8.735	25.177	1.00	39.59
ATOM ATOM	5313	CE3	TRP	684	45.869	8.416.		1.00	39.26
ATOM	5314 5315	CD1 NE1	TRP	684	47.842	8.373	24.528	1.00	39.02
ATOM	5315	CZ2	TRP TRP	684 684	46.576 44.362	8.687	24.096	1.00	38.42
ATOM	5317	CZ3	TRP	684	44.502	9.011	25.240	1.00	36.62
ATOM	5319	CH2	TRP	684	43.766	8.691 8.982	27.641	1.00	40.70
ATOM	5320	C	TRP	684	49.819	6.158	26.475 25.125	1.00	40.57 31.98
ATOM	5321	ō	TRP	684	49.066	5.367	24.557	1.00	32.43
ATOM	5322	N	SER	685	50.859	6.748	24.529	1.00	29.63
ATOM	5324	CA	SER	685	51.195	6.531	23.119	1.00	28.62
ATOM	5325	CB	SER	685	52.457	7.296	22.751	1.00	24.72
ATOM	5326	OG	SER	685	52.323	8.664	23.072	1.00	30.04
ATOM	5328	C	SER	685	51.414	5.055	22.825	1.00	27.91
ATOM	5329	0	SER	685	51.022	4.555	21.767	1.00	28.60
ATOM	5330	N	PHE	686	52.063	4.372	23.763	1.00	27.96
ATOM	5332	CA	PHE	686	52.333	2.947	23.662	1.00	27.03
ATOM	5333	CB	PHE	686	53.163	2.499	24.868	1.00	25.79
ATOM	5334	CG	PHE	686	53.440	1.029	24.890	1.00	26.25
ATOM	5335	CD1	PHE	686	<b>54.2</b> 52	0.451	23.923	1.00	27.32
MOTA	5336	CD2	PHE	686	52.839	0.208	25.841	1.00	26.22
ATOM	5337	CEl	PHE	686	54.464	-0.930	23.900	1.00	25.87
ATOM	5338	CE2	PHE	686	53.046	-1.170	25.828	1.00	24.37
MOTA	5339	CZ	PHE	686	53.856	-1.740	24.854	1.00	26.42
MOTA	5340	С	PHE	686	51.003	2.160	23.596	1.00	28.82
ATOM	5341	0	PHE	686	50.912	1.129	22.914	1.00	26.74
MOTA	5342	N	GLY	687	49.991	2.636	24.324	1.00	29.52

							1	.86				
	MOT	5344	CA	GLY	687							
		5345	С	GLY	687		688	1.	982	24.302	1.00	22.5-
	MO	5346	0	GLY			095	2.		22.896	1.00	
AT		5347	N	VAL	687	- ' •			_	22.414		. •
AT		5349	CA	VAL	688	48.				22.238	1.00	29.83
AT		350	СВ		688	47.			_	20.879	1.00	29.06
ATO		351	CG1	VAL	688	47.8	300			0.424	1.00	28.93
ATO		352		VAL	688	47.2	211			0.424	1.00	27.24
ATO		353	CG2	VAL	688	46.9	90			9.020	1.00	28.29
ATC		~ - :	_	VAL	688	48.6	12	2.4		1.404	1.00	26.96
ATO	_			VAL	688	48.0	80	1.8		9.951	1.00	28.49
ATO		~		LEU	689	49.9	05			9.024	1.00	28.84
ATO				LEU	689	50.8	04	2.3		0.252	1.00	27.99
				LEU	689	52.2	60	1.5		9.461	1.00	26.14
ATO		359 (	CG 1	LEU	689	53.3	C D	1.6		9.911	1.00	27.31
ATO					689	53.30	58	1.0	14 19	.065	1.00	26.60
ATO					689	54.68	38	1.7	57 19	1.175	1.00	
ATOM		62 C	_		689	53.56		-0.40	01 19	.475	1.00	28.19
ATOM	1 53	63 O	_			50.36		0.09		.605		25.55
ATOM	1 53				589	50.37		-0.68		.626	1.00	26.48
ATOM	1 53				90	49.95	3	-0.34		.816	1.00	27.06
ATOM	53				90	49.46	5	-1.70	_	_	1.00	28.55
ATOM	536		_		90	49.07	0	-1.88			1.00	29.16
ATOM				_	90	50.11		-2.08			1.00	31.40
ATOM					90	49.42		-2.02		667	1.00	31.49
ATOM				-	90	50.82		-3.41		026	1.00	34.09
ATOM		_	LE	TU 6	90	48.240		3.4T		491		30.84
ATOM	537	_	LE	U 6	90	48.088		-1.95		220 ]	1.00	26.51
ATOM	537		TR	P 69	91	47.376		-3.023		631 <u>1</u>		25.15
ATOM	537			P 69	91	46.169		-0.954		139 1		8.51
	537		TR	P 69	1	45.332		-1.049				9.56
ATOM	537	_	TR			43.992		0.227		465 <u>1</u>	.00 2	8.91
ATOM	5378		2 TR					0.169				0.95
ATOM	5379	CE:	TRI			43.718		0.556	17.4			9.87
ATOM	5380					42.337		0.367	17.1			
ATOM	5381	CD1				44.505		1.049	16.3			1.97
ATOM	5382					42.796		0.231	19.2			7.72
ATOM	5384	CZ2				41.797	-	0.111	18.3			0.68
ATOM	5385					41.729		0.652	15.9			3.68
MOTA	5386	CH2	TRP			43.906		1.327	15.1			.42
MOTA	5387	C	TRP	691		42.523		l.129	14.9			.13
ATOM	5388	ō		691		46.564		.289	17.8		• •	.18
ATOM	5389	_	TRP	691		45.996	- 2	1.156			_	. 78
	5391	N	GLU	692		47.564	- 0	.543	17.19	<del></del>		. 64
	5392	CA	GLU	692		48.078	- 0	.669	17.38	_		. 83
<b>&gt;</b>	5393	CB	GLU	692		49.267		.262	16.01		00 28	. 08
3		CG	GLU	692		48.945	1	.735	15.79		00 26	40
	5394	CD	GLU	692		50.183	7	. /35	15.68	0 1.0	00 26	
	5395	OE1	GLU	692		50.938		. 561	15.36	9 1.0	0 29.	
3	5396	OE2	GLU	692	2	0.413		. 886	16.32	0 1.0		
	5397	C	GLU	692	-	0 500		. 875	14.18	2 1.0		
ATOM 5	398	0	GLU	692		8.563		082	15.76			7.7 0.7
	399	N	ILE			8.385		612	14.669		•	υ / 3.0
30000	401	CA	ILE	693	4	9.244		663	16.746			7 R
ATOM 5	402	CB	ILE	693		9.754			16.608	_		
30000	403	CG2		693		0.632			17.828	-		
	404	CG1	ILE	693		1.037			17.706			
		CGI	ILE	693	5.	1.907	-3.		17.890			
SSSD/5514	5 001						•		÷ / . 0 9 U	1.00	26.9	9
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ATOM	5405	CD1	ILE	693	52.663	-3.747	19.194	1.00	25.37
ATOM	5406	С	ILE	693	48.603	-5.023	16.452	1.00	29.21
ATOM	5407	0	ILE	693	48.568	-5.807	15.512	1.00	27.89
ATOM	1 5408	N	PHE	694	47.623	-4.942	17.336	1.00	31.33
ATOM	5410	CA	PHE	694	46.523	-5.888	17.279	1.00	34.41
ATOM	5411	СВ	PHE	694	45.958	-6.114	18.687	1.00	35.37
ATOM	5412	CG	PHE	694	46.978	-6.717	19.621	1.00	35.60
ATOM	5413	CD1	PHE	694	47.606	-5.942	20.586	1.00	37.23
MOTA	5414	CD2	PHE	694	47.424	-8.024	19.426	1.00	35.59
ATOM		CEl	PHE	694	48.669	-6.460	21.333	1.00	36.39
ATOM		CE2	PHE	694	48.484	-8.546	20.170	1.00	35.34
ATOM		CZ	PHE	694	49.110	-7.762	21.118	1.00	35.71
ATOM		C	PHE	694	45.481	-5.715	16.176	1.00	34.41
ATOM		0	PHE	694	44.623	-6.579	15.982	1.00	34.48
ATOM		N	THR	695	45.617	-4.637	15.404	1.00	33.03
ATOM		CA	THR	695	44.742	-4.379	14.263	1.00	31.81
ATOM		CB	THR	695	44.113	-2.957	14.278	1.00	29.75
ATOM		OG1	THR	695	45.142	-1.961	14.218	1.00	30.72
ATOM		CG2	THR	695	43.254	-2.759	15.524	1.00	
ATOM		C	THR	695	45.596				29.40
ATOM		0	THR	695		-4.533	13.011	1.00	31.44
ATOM					45.153	-4.241	11.906	1.00	33.00
ATOM		N	LEU	696	46.832	-4.987	13.209	1.00	31.24
		CA	LEU	696	47.799	-5.199	12.134	1.00	31.36
ATOM		CB	LEU	696	47.421	-6.418	11.291	1.00	33.53
ATOM		CG	LEU	696	47.270	-7.741	12.042	1.00	33.00
MOTA		CD1	LEU	696	47.010	-8.838	11.052	1.00	35.50
MOTA		CD2	LEU	696	48.515	-8.061	12.830	1.00	36.09
ATOM		C	LEU	696	48.066	-3.976	11.249	1.00	30.84
ATOM		0	LEU	696	48.135	-4.067	10.024	1.00	28.23
ATOM		N	GLY	697	48.302	-2.839	11.890	1.00	31.54
ATOM		CA	GLY	697	48.591	-1.632	11.141	1.00	33.87
ATOM		C	GLY	697	47.375	-0.765	10.924	1.00	32.77
ATOM		0	GLY	697	47.322	0.042	9.994	1.00	33.90
ATOM		N	GLY	698	46.392	-0.921	11.797	1.00	33.29
ATOM		CA	GLY	698	45.187	-0.122	11.681	1.00	32.66
ATOM		C	GLY	698	45.408	1.368	11.877	1.00	30.57
ATOM		0	GLY	698	46.336	1.803	12.553	1.00	27.36
ATOM		N	SER	699	44.517	2.148	11.285	1.00	30.92
MOTA		CA	SER	699	44.552		11.376	1.00	32.19
ATOM		CB	SER	699	44.062	4.202	10.058	1.00	34.24
ATOM		OG	SER	699	44.019	5.616	10.123	1.00	38.67
ATOM		С	SER	699	43.644	4.014	12.538	1.00	31.81
MOTA		0	SER	699	42.431	3.759	12.525	1.00	31.39
ATOM		N	PRO	700	44.228	4.597	13.594	1.00	31.82
ATOM		CD	PRO	700	45.645	4.842	13.919	1.00	28.82
MOTA	5458	CA	PRO	700	43.353	4.992	14.697	1.00	31.31
ATOM	5459	CB	PRO	700	44.345	5.341	15.809	1.00	31.31
ATOM	5460	CG	PRO	700	45.552	5.800	15.061	1.00	30.41
ATOM	5461	С	PRO	700	42.484	6.170	14.295	1.00	31.19
ATOM	5462	0	PRO	700	42.899	7.021	13.510	1.00	29.93
ATOM	5463	N	TYR	701	41.235	6.144		1.00	32.69
ATOM	5465	CA	TYR	701	40.291	7.223	14.445	1.00	32.54
ATOM		CB	TYR	701	40.650	8.416	15.323	1.00	34.47
ATOM	5467	CG	TYR	701	40.512	8.141	16.794	1.00	39.16

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A	TOM	5468	CD1	TYR	701		0.2				
		5469	CE1	TYR	701			433 17	. 683	1.00	44.31
A'	TOM 5	470	CD2	TYR		0				1.00	
A'		471	CE2		701		21 7.			1.00	46.65
A.		472		TYR	701	39.1					41.21
	_	473	CZ	TYR	701	40.16				.00	45.05
			OH	TYR	701	39.94				.00	47.24
			С	TYR	701	40.21		•		.00	52.18
			О	TYR	701	40.37		_		.00	30.56
			N	PRO	702	39.92				.00	29.73
		478	CD :	PRO	702	39.65				.00	30.38
		179 (	CA :	PRO	702				261 1	.00	30.22
TA	OM 54	80 (		PRO	702	39.84			_	.00	28.87
AT	OM 54	81 (		PRO	702	39.69		22 9.9		. 00	.29.63
ATC		82 (		PRO		39.00		89 10.9		.00	
ATO		83 0			702	38.72		48 10.2			30.99
ATO		84 N	_	RO	702	37.557	7 7.84			00	30.88
ATC				LY	703	39.100	9.1			00	33.98
ATC				LY	703	38.154	10.13			00	29.03
	M . 54		_		703	37.893				00	28.98
ATO			_	LY	703	37.074				00	29.69
ATO			V	AL	704	38.579				00	31.71
			A V	AL '	704	38.416		_			30.74
ATO		- 0.	S V	AL '	704	38.582				0 C	32.06
ATO			31 V <i>j</i>	TT :	704	38.522					31.70
ATO		4 CG	32 V		704	37.506	12.19				30.29
ATO		5 C	VA		704		10.14		5 1.0		31.56
ATON		6 0	VA		04	39.430	13.08		9 1.0		33.72
ATON		7 N	PR	_	05	40.634	12.86	7 12.54	8 1.0		35.31
ATOM		8 CD			05	38.957	14.309	12.20			34.23
ATOM						37.594	14.692	11.78		_	
ATOM	550				05	39.875	15.443	12.13			3.20
ATOM					05	39.053	16.495			_	3.73
ATOM			PRO		05	37.647	16.187				4.93
ATOM			PRO		05	40.280	15.879		-		6.93
ATOM		_	PRO		05	39.651	15.490				3.25
ATOM	5506		VAI		06	41.322	16.697		-		1.71
ATOM	5507		VAI		6	41.852	17.176				4.46
ATOM			VAL	, 70	6	42.923	18.261	14.900			5.99
ATOM	5508			70	6	43.577	18.618	14.687			9.01
ATOM	5509		VAL	70	6	43.961	17.786	16.017	-		.33
ATOM	5510		VAL	70	6	40.826		13.673			.61
	5511	0	VAL	70	6	40.823	17.716	15.895	1.00		.65
ATOM	5512	N	GLU			39.955	17.319	17.065	1.00		.55
ATOM	5514	CA	GLU			38.941	18.605	15.426	1.00		. 74
ATOM	5515	CB	GLU	70		30.341	19.220	16.27B	1.00		.20
MOTA	5516	C	GLU	70		38.129	20.242	15.482	1.00		. 98
ATOM	5517	0	GLU	70		38.014	18.188	16.900	1.00		.46
ATOM	5518	N	GLU			37.634	18.295	18.074	1.00		
ATOM	5520	CA		708		37.681	17.170	16.115	1.00		. 04
ATOM	5521	CB	GLU	708		36.802	16.105	16.571	1.00		. 81
ATOM	5522		GLU	708		36.316	15.289	15.378		37.	
ATOM	5523	CG	GLU	708		35.459	16.091	14.413	1.00	40.	
ATOM		CD	GLU	708		34.235	16.677		1.00	43.	
ATOM	5524	OE1	GLU	708		33.629	16.007	15.084	1.00	51.	
	5525	OE2	GLU	708		33.882		15.961	1.00	50.	
ATOM	5526	C	GLU	708		37.506	17.824	14.732	1.00	59.	
ATOM	5527	0	GLU	708		36.897	15.223	17.588	1.00	36.	
CCC - :					•		14.782	18.567	1.00	36.	
SSSD/55	145. v01										

ATOM	5528	N	LEU	709	38.799	14.993	17.376	1.00	35.69
ATOM	5530	CA	LEU	709	39.584	14.179	18.301	1.00	35.48
ATOM	5531	CB	LEU	709	41.039	14.044	17.830	1.00	34.84
ATOM	5532	CG	LEU	709	41.921	13.250	18.802	1.00	32.41
ATOM	5533	CD1	LEU	709	41.608	11.787	18.674	1.00	30.10
ATOM	5534	CD2	LEU	709	43.378	13.514	18.560	1.00	29.93
ATOM	5535	С	LEU	709	39.568	14.842	19.673	1.00	35.58
ATOM	5536	0	LEU	709	39.377	14.177	20.694	1.00	35.43
ATOM	5537	N	PHE	710	39. <b>7</b> 92	16.150	19.686	1.00	36.79
ATOM	5539	CA	PHE	710	39.800	16.918	20.927	1.00	40.58
ATOM	5540	CB	PHE	710	39.944	18.413	20.637	1.00	
MOTA	5541	CG	PHE	710	41.308	18.808	20.162	1.00	46.38
ATOM	5542	CD1	PHE	710	42.392	17.942	20.313	1.00	47.29
ATOM	5543	CD2	PHE	710	41.515	20.050	19.580	1.00	47.93
ATOM	5544	CE1	PHE	710	43.659	18.312	19.892	1.00	51.21
ATOM	5545	CE2	PHE	710	42.781	20.435	19.155	1.00	50.89
ATOM	5546	CZ	PHE	710	43.859	19.562	19.312	1.00	53.31
ATOM	5547	С 0	PHE	710	38.517	16.676	21.694	1.00	40.14
ATOM ATOM	5548 5549	N	PHE LYS	710 711	38.543 37.399	16.446 16.705	22.898	1.00	39.86
ATOM	5551	CA	LYS	711	36.101	16.479	20.977 21.584	1.00	41.02
ATOM	5552	CB	LYS	711	34.985	16.803	20.580	1.00	38.66 40.75
ATOM	5553	CG	LYS	711	33.601	16.727	21.181	1.00	46.99
ATOM	5554	CD	LYS	711	32.522	17.174	20.218	1.00	50.71
ATOM	5555	CE	LYS	711	31.163	16.733	20.739	1.00	52.53
ATOM	5556	NZ	LYS	711	30.041	17.194	19.884	1.00	57.76
ATOM	5560	C	LYS	711	35.990	15.046	22.120	1.00	38.06
ATOM	5561	0	LYS	711	35.535	14.831	23.250	1.00	36.29
ATOM	5562	N	LEU	712	36.431	14.066	21.330	1.00	38.10
ATOM	5564	CA	LEU	712	36.392	12.662	21.764	1.00	38.69
ATOM	5565	CB	LEU	712	36.914	11.714	20.672	1.00	37.19
ATOM	5566	CG	LEU	712	36.070	11.436	19.424	1.00	34.73
ATOM	5567	CD1	LEU	712	36.814	10.453	18.524	1.00	35.54
ATOM	5568	CD2	LEU	712	34.709	10.872	19.818	1.00	30.90
ATOM	5569	C	LEU	712	37.230	12.472	23.021	1.00	39.62
MOTA	5570	0	LEU	712	36.843	11.745	23.940	1.00	39.44
ATOM	5571	N	LEU	713	38.398	13.101	23.044	1.00	40.10
MOTA	5573	CA	LEU	713	39.279	12.999	24.199	1.00	42.81
ATOM	5574	CB	LEU	713	40.606	13.716	23.924	1.00	41.70
ATOM	5575	CG	LEU	713	41.495	13.040	22.868	1.00	41.86
ATOM	5576	CD1	LEU	713	42.742	13.862	22.607	1.00	37.19
ATOM	5577	CD2	LEU	713	41.873	11.647	23.340	1.00	41.17
ATOM	5578	C	LEU	713	38.577	13.566	25.437	1.00	43.18
MOTA	5579	0	LEU	713	38.479	12.889	26.457	1.00	44.79
ATOM	5580	N	LYS	714	38.004	14.760	25.312	1.00	42.75
ATOM	5582	CA	LYS	714	37.301	15.389	26.425	1.00	43.70
MOTA	5583	CB	LYS	714	36.842	16.796	26.043	1.00	44.69
ATOM	5584	CG	LYS	714	38.001	17.746	25.836	1.00	47.92
ATOM	5585 5586	CD	LYS	714	37.543	19.171	25.583	1.00	55.01
ATOM ATOM	5586 5587	CE NZ	LYS LYS	714 714	38.733	20.077	25.238	1.00	59.44
ATOM	5591	C C	LYS	714	39.773 36.127	20.132	26.320	1.00	60.10
ATOM	5592	0	LYS	714	35.843	14.557 14.551	26.940 28.140	1.00	43.94 44.20
ATOM	5592 5593	N	GLU	715	35.477				
ATOM	2223	7.4	GLU	113	33.4//	13.819	26.046	1.00	43.29





•					-
			190		
ATOM 5595	CA GLU	71-			
ATOM 5596	CB GLU	715 34.		9 26 425	
ATOM 5597	CG GLU	715 33.4	164 12.68		1.00 42.29
ATOM 5598	910	715 32.9	13 13.916		1.00 44.91
ATOM 5599	010	715 32.0	13.566		1.00 51.62
ATOM 5600	221 GTO	715 32.3			1.00 55.01
ATOM 5601	OE2 GLU	715 30.9			1.00 58.09
	C GLU	715 34.8			
3.000-	A			27.064	
100	<b>&gt;</b> 2			2 -	,
ATOM 5605	CA		lB 11.476	<b>~</b>	1.00 38.01
ATOM 5606	C 07.1-	50.04	10.252	0	1.00 41.11
ATOM 5607	0 ~	16 36.51	.0 9.054	2 -	1.00 39.69
ATOM 5608	N	16 36.56	2 7.904		1.00 39.64
ATOM 5610	CA ****	<sup>17</sup> 36.35	9 9.335		.00 36.71
ATOM 5611	~	17 36.21		25.554 1	.00 41.95
ATOM 5612		35.85		24.541 1	.00 43.32
3000	CG HIS 71	35.81		23.183 1	.00 43.38
	CD2 HIS 71	.7 34.802			
	ND1 HIS 71			22	
T Most	CE1 HIS 71	512		21 200	
_ ·	NE2 HIS 71			20	-0.21
	C HIS 71	55.307	6.404	2.0	00 46.21
ATOM 5620	O HIS 71	27.403	7.481	24	00 45.55
ATOM 5621 1	NT	00.561	8.031	24 -	00 43.90
ATOM 5623 (	77	57.304		O	00 45.45
ATOM cca.	716	50.36/		24.289 1.	00 43.44
ATOM CCO.	70 718	38.500		24.139 1.	00 42.68
ATOM CCC		38.844	_	25.412 1.0	00 41.00
ATOM SCOR	D ARG 718	40.214	5.165	<sup>26.658</sup> 1.0	
ATOM Econ	E ARG 718	40.658	5.825	<sup>26</sup> .495 1.0	
ATOM -	/1K	40.521	6.549	27.685 1.0	
ATOM SSS	H1 ARG 718	39.940	7.861 2	7.862 1.0	
30000	H2 ARG 718	41 004	8.608 2	6.931 1.0	
	ARG 718	41.024	8.443 2	8.946 1.0	
ATOM 5637 O	ARG 718	38.080	4.308 2	_	
ATOM 5638 N	MET 719	36.911		<b>^</b>	· <del>-</del>
ATOM 5640 CA		39.113	_		
ATOM 5641 CB	1121 /19	38.928	_		
ATOM 5642 CG	/19	40.219	_	1.004 1.00	
ATOM 5643 SD	719	40.595		1.00	42.59
ATOM 5644 CE	MET 719	42.093	4 4	1.413 1.00	41.15
ATOM CC.	MET 719	43.323	• -	.400 1.00	44.11
ATOM CC.	MET 719	38.460	_	.613 1.00	41.33
ATOM CC.	MET 719	38.822	1.694 21	.432 1.00	44.74
ATOM ST.	ASP 720	37.635	1.216 22	.516 1.00	41.56
LA CA	ASP 720	37.000	1.075 20	.582 1.00	
June CD	ASP 720	37.090	~0.265 20	824 1.00	45.50
ATOM 5651 CG	ASP 720	36.077			45.51
ATOM 5652 OD1		34.811		_	48.60
ATOM 5653 OD2		34.678			53.03
ATOM 5654 C		33.943	_	612 1.00	59.61
ATOM 5655 O	ASP 720			880 1.00	50.58
ATOM SCSS	ASP 720		_	823 1.00	43.64
ATOM FOR	LYS 721		1.172 20.	199 1.00	43.66
ATOM SSE	LYS 721		2.436 21.4	187 1.00	
	LYS 721	~ ~	·3·565 21 i	555 1.00	42.90
	LYS 721	38.278 _	4.565 22.5	1.00	42.96
ATOM 5661 CD	LYS 721	39.000 -	5.888 22.5	7.0	42.51
-	121	38.445 -	6.805 23.6	20	47.68
SSSD/55145. v01			~~.0	28 1.00	51.61





ATOM	5662	CE	LYS	721	38.450	-8.246	23.163	1.00	54.96	
ATOM	5663	NZ	LYS	721	38.165	-9.190	24.282	1.00	59.67	
MOTA	5667	C	LYS	721	38.825	-4.215	20.182	1.00	43.05	
MOTA	5668	0	LYS	721	37.779	-4.577	19.625	1.00	46.08	
ATOM	5669	N	PRO	722	40.025	-4.348	19.601	1.00	43.22	
ATOM	5670	CD	PRO	722	41.337	-3.872	20.067	1.00	43.52	
ATOM	5671	CA	PRO	722	40.139	-4.968	18.275	1.00	41.04	
ATOM	5672	CB	PRO	722	41.631	-4.856	17.965	1.00	40.87	
ATOM	5673	CG	PRO	722	42.074	-3.682	18.764	1.00	42.22	
ATOM	5674	C	PRO	722	39.726	-6.427	18.346	1.00	39.64	
ATOM	5675	0	PRO	722	39.730	-7.023	19.425	1.00	37.12	
ATOM	5676	N	SER	723	39.311	-6.982	17.212	1.00	40.36	
ATOM	5678	CA	SER	723	38.947	-8.389	17.158	1.00	41.41	
ATOM	5679	CB	SER	723	38.205	-8.707	15.865	1.00	38.26	
ATOM	5680	OG	SER	723	39.049	-8.520	14.749	1.00	43.87	
ATOM	5682	С	SER	723	40.294	-9.102	17.191	1.00	41.54	
ATOM	5683	0	SER	723	41.284	-8.575	16.703	1.00	40.90	
MOTA	5684	N	ASN	724	40.338	-10.300	17.750	1.00	44.89	
ATOM	5686	CA	ASN	724	41.598	-11.019	17.853	1.00	48.14	
ATOM	5687	CB	ASN	724	42.256	-11.202	16.476	1.00	52.43	
MOTA	5688	CG	ASN	724	41.682	-12.374	15.715	1.00	57.29	
MOTA	5689	OD1	ASN	724	41.637	-13.492	16.225	1.00	61.96	
ATOM	5690	ND2	ASN	724	41.218	-12.125	14.500	1.00	60.91	
ATOM	5693	С	ASN	724	42.509	-10.255	18.811	1.00	48.17	
ATOM	5694	0	ASN	724	43.648	-9.918	18.495	1.00	49.88	
ATOM	5695	N	CYS	725	41.960	-9.935	19.973	1.00	47.12	
ATOM	5697	CA	CYS	725	42.686	-9.238	21.010	1.00	46.17	
ATOM	5698	CB	CYS	725	42.569	-7.717	20.862	1.00	44.83	
ATOM	5699	SG	CYS	725	43.459	-6.813	22.159	1.00	42.51	
MOTA	5700	C	CYS	725	42.017	-9.697	22.294	1.00	45.78	
ATOM	5701	0	CYS	725	40.803	-9.642	22.423	1.00	44.83	
ATOM	5702	N	THR	726	42.810	-10.224	23.212	1.00	45.63	
ATOM	5704	CA	THR	726	42.289	-10.711	24.482	1.00	45.47	
ATOM	5705	CB	THR	726	43.351	-11.545	25.217	1.00	45.93	
ATOM	5706	OG1	THR	726	44.307	-10.651	25.786	1.00	45.04	
MOTA	5708	CG2	THR	726	44.061	-12.495	24.233	1.00	42.99	
MOTA	5709	С	THR	726	41.858	-9.545	25.359	1.00	45.73	
ATOM	5710	0	THR	726	42.368	-8.445	25.216	1.00	46.91	
ATOM	5711	N	ASN	727	40.914	-9.789	26.257	1.00	45.93	
MOTA	5713	CA	ASN	727	40.448	-8.736	27.141	1.00	47.85	
ATOM	5714	CB	ASN	727	39.300	-9.237	28.022	1.00	54.88	
MOTA	5715	CG	ASN	727	39.629	-10.544	28.731	1.00	65.11	
MOTA	5716	OD1	asn	727	40.737	-10.734	29.229	1.00	70.58	
ATOM	5717	ND2	ASN	727	38.681	-11.472	28.735	1.00	69.68	
MOTA	5720	C	ASN	727	41.591	-8.212	27.999	1.00	44.18	
MOTA	5721	0	ASN	727	41.594	-7.047	28.390	1.00	41.35	
ATOM	5722	N	GLU	728	42.572	-9.073	28.260	1.00	42.82	
ATOM	5724	CA	GLU	728	43.725	-8.713	29.071	1.00	42.37	
ATOM	5725	CB	GLU	728	44.573	-9.952	29.379	1.00	43.09	
MOTA	5726	CG	GLU	728	45.806	-9.654	30.245	1.00	48.30	
ATOM	5727	CD	GLU	728	46.643	-10.889	30.568	1.00	50.11	
MOTA	5728	OE1	GLU	728	46.867	-11.732	29.668	1.00	47.98	
MOTA	5729	OE2	GLU	728	47.085	-11.010	31.733	1.00	51.69	
ATOM	5730	C	GLU	728	44.551	-7.652	28.356	1.00	39.57	





		5731	0	GLU	728	44.6					
		5732	N	LEU	729	44.8	-	.605 28	3.933	1.00	30.20
		5734	CA	LEU	729	• •		.907 27	.089	1.00	39.30
		5735	CB	LEU	729	45.6	55 ~6		. 274	1.00	37.38
		736	CG	LEU	729	46.02			. 935	1.00	36.74
		737	CD1	LEU		47.13			.001	1.00	35.39
A	TOM 5	738	CD2	LEU	729	47.10	)7 -9.		. 766		35.41
A		739	C		729	48.50	95 -8.	_	.174	1.00	35.69
A <sup>c</sup>		740	_	LEU	729	44.88				1.00	37.72
				LEU	729	45.46				1.00	35.52
		<b>.</b>		TYR	730	43.56				1.00	33.96
				TYR	730	42.76				1.00	32.90
				TYR	730	41.33	- • .			1.00	32.41
		<b>.</b>		<b>TYR</b>	730	40.44			398 1	1.00	32.16
				ľYR	730	40.769			172 1	.00	34.93
		47 (	CE1 7	'YR	730	39.962		-		.00	32.49
AT			D2 1		730				^ ^ .		32.80
AT		49 C	E2 1		730	39.282					33.45
AT		50 C			730	38.465		96 25.			
ATO		51 0			730	38.814		57 24.7			34.81
ATO	DM 57.	53 C	_			38.009		65 24.5			34.06
ATC	DM 57		-		730	42.767	-3.7		_		36.66
ATO	M 575		•		730	42.837	-2.5			.00 3	3.48
ATO			_ • • •	'	731	42.698	-4.46			.00 3	4.94
ATO			_		31	42.724	-3.75				5.29
ATO					31	42.465	-4.70				8.38
ATO					31	41.048	~5.26			00 4	2.01
ATO				-	31	39.785	-3.96	• •		00 5	3.67
ATO			ME.	T 7	31	39.828				00 6	2.97
ATON		_	ME	T 7:	31	44.073	-3.68				1.83
ATOM			ME	T 73	31	44.160	-3.04			00 34	1.52
ATOM			ME	T 73	32	45.118	-1.95		2 . 1.(		3.23
			ME'	Г 73	32	46.445	-3.66		4 1.0		. 93
ATOM			ME'			47.506	-3.069		8 1.0		.26
ATOM	-		MET			48.935	-3.999		5 1.0		. 56
ATOM	-		MET			70.935 FO 706	-3.418		3 1.0	_	.26
ATOM			MET			50.186	-4.522		1 1.0		.46
ATOM			MET			50.480	-5.562	29.41		_	
ATOM	5772	0	MET	. •		46.369	-1.750	28.389		_	. 88
ATOM	5773	N	MET			46.827	-0.722	28.873			. 75
ATOM	5775	CA	MET	733	_	45.741	-1.774	27.213			49
ATOM	5776	CB	MET			45.571	-0.566	26.413	1.00		
ATOM	5777	CG	MET	733		44.787	-0.853	25.130	1.00		
MOTA	5778	SD		733		45.544	-1.601	24.047		٠.	16
ATOM	5779	CE	MET	733		44.421	-1.990	22.670			
ATOM	5780	CE	MET	733		45.155	-3.496	22.670	1.00		66
ATOM	5781		MET	733		14.789	0.452	22.068	1.00		47
ATOM		0	MET	733		15.176	1.619	27.229	1.00		94
ATOM	5782	N	ARG	734		13.679	1.019	27.318	1.00	35.	
	5784	CA	ARG	734	4	2.854	0.018	27.818	1.00		
ATOM	5785	CB	ARG	734	4	1.586	0.913	28.621	1.00	33.4	
ATOM	5786	CG	ARG	734			0.197	29.095	1.00	33.4	
ATOM	5787	CD	ARG	734		0.726	-0.335	27.950	1.00	34.2	
ATOM	5788	NE	ARG	734		0.256	0.783	27.043	1.00		
ATOM	5790	CZ	ARG			9.416	1.745	27.750	1.00	37.7	
ATOM	5791	NH1	ARG	734		8.092	1.661	27.844		43.9	
ATOM	5794	NH2		734		7.439	0.660	27.268	1.00	46.4	
		-4112	ARG	734	3.	7.420	2.571	28.530	1.00	48.6	
SSSD/551	145 201							~0.330	1.00	44.6	5

ATOM	5797	С	ARG	734	43.660	1.458	29.793	1.00	32.12
MOTA	5798	0	ARG	734	43.492	2.610	30.180	1.00	35.37
MOTA	5799	N	ASP	735	44.566	0.646	30.327	1.00	33.75
MOTA	5801	CA	ASP	735	45.438	1.076	31.433	1.00	36.72
ATOM	5802	CB	ASP	735	46.379	-0.055	31.857	1.00	42.71
MOTA	5803	CG	ASP	735	45.722	-1.052	32.774	1.00	47.31
ATOM	5804	OD1	ASP	735	46.124	-2.241	32.720	1.00	50.99
MOTA	5805	OD2	ASP	735	44.824	-0.646	33.552	1.00	48.45
MOTA	5806	C	ASP	735	46.291	2.251	30.972	1.00	34.25
MOTA	5807	0	ASP	735	46.376	3.286	31.648	1.00	34.31
ATOM	5808	N	CYS	736	46.927	2.064	29.816	1.00	31.85
ATOM	5810	CA	CYS	736	47.780	3.077	29.204	1.00	29.93
MOTA	5811	CB	CYS	736	48.413	2.545	27.921	1.00	24.97
MOTA	5812	SG	CYS	736	49.504	1.159	28.180	1.00	31.35
MOTA	5813	C	CYS	736	46.994	4.325	28.885	1.00	31.62
MOTA	5814	0	CYS	736	47.562	5.416	28.823	1.00	30.73
ATOM	5815	N	TRP	737	45.680	4.174	28.711	1.00	35.03
MOTA	5817	CA	TRP	737	44.812	5.308	28.395	1.00	36.35
ATOM	5818	CB	TRP	737	43.808	4.927	27.297	1.00	36.43
MOTA	5819	CG	TRP	737	44.451	4.487	26.010	1.00	34.34
MOTA	5820	CD2	TRP	737	43.914	3.565	25.052	1.00	34.81
MOTA	5821	CE2	TRP	737	44.852	3.461	23.999	1.00	33.92
MOTA	5822	CE3	TRP	737	42.730	2.816	24.980	1.00	33.06
ATOM	5823	CD1	TRP	737	45.659	4.890	25.514	1.00	35.19
MOTA	5824	NE1	TRP	737	45.907	4.279	24.309	1.00	35.00
MOTA	5826	CZ2	TRP	737	44.644	2.633	22.886	1.00	33.45
MOTA	5827	CZ3	TRP	737	42.527	1.991	23.876	1.00	32.92
MOTA	5828	CH2	TRP	737	43.480	1.909	22.844	1.00	30.45
MOTA	5829	C	TRP	737	44.080	5.895	29.609	1.00	37.23
ATOM	5830	0	TRP	737	43.047	6.551	29.474	1.00	37.44
MOTA	5831	N	HIS	738	44.624	5.681	30.798	1.00	41.45
ATOM	5833	CA	HIS	738	44.006	6.208	32.008	1.00	41.52
MOTA	5834	CB	HIS	738	44.675	5.635	33.258	1.00	41.23
MOTA	5835	CG	HIS	738	43.925	5.924	34.522	1.00	43.31
MOTA	5836	CD2	HIS	738	43.618	7.096	35.126	1.00	41.58
MOTA	5837	ND1	HIS	738	43.338	4.935	35.279	1.00	44.22
MOTA	5839	CEl	HIS	738	42.693	5.487	36.294	1.00	46.62
ATOM	5840	NE2	HIS	738	42.848	6.798	36.223	1.00	43.99
ATOM	5842	C	HIS	738	44.118	7.726	32.015	1.00	41.75
ATOM	5843	0	HIS	738	45.179	8.268	31.731	1.00	40.84
MOTA	5844	N	ALA	739	43.025	8.405	32.352	1.00	42.47
ATOM	5846	CA	ALA	739	43.004	9.873	32.398	1.00	44.58
MOTA	5847	CB	ALA	739	41.629	10.361	32.825	1.00	48.19
MOTA	5848	С	ALA	739	44.081	10.467	33.317.	1.00	45.12
MOTA	5849	0	ALA	739	44.653	11.510	33.020	1.00	45.66
MOTA	5850	N	VAL	740	44.262	9.852	34.481	1.00	46.64
MOTA	5852	CA	VAL	740	45.278	10.273	35.453	1.00	46.78
MOTA	5853	CB	VAL	740	44.867	9.893	36.888	1.00	47.74
ATOM	5854	CG1	VAL	740	45.919	10.372	37.890	1.00	49.35
MOTA	5855	CG2	VAL	740	43.515	10.495	37.211	1.00	47.89
MOTA	5856	С	VAL	740	46.601	9.573	35.121	1.00	45.24
MOTA	5857	0	VAL	740	46.754	8.362	35.347	1.00	45.01
MOTA	5858	N	PRO	741	47.588	10.335	34.637	1.00	43.46
MOTA	5859	CD	PRO	741	47.536	11.794	34.437	1.00	43.51

AT	'OM 5	860	CA	PRO :	741						
AT	OM 5	861	CB		741	48.90	_	.804	4.266	1.00	46 22
AT	OM 5	862	CG		41	49.70			3.942	1.00	
ATO		863	_		41	48.63			3.426	1.00	
ATO		364	_	`		49.58			5.328	1.00	
ATC				-	41	50.24			4.994	1.00	47.45
ATC	DM 58		'		42	49.39	49.		6.601		45.12
ATO					42	49.99	1 8.		7.703	1.00	48.78
ATO					42	49.845	5 9.		9.012	1.00	48.76
ATO	M 58	_			12	48.482	9.		9.373	1.00	51.11
ATO		-	. 7		12	49.376			7.867	1.00	53.50
ATO:				ER 74		49.932				1.00	47.77
ATO				LN 74	3	48.199			3.539	1.00	47.31
ATON			_	LN 74	3	47.511			284	1.00	47.57
ATON				LN 74		46.004	5.9		.384	1.00	47.14
ATOM		_		LN 74	3	45.438			.531	1.00	50.16
ATOM	,			LN 74	3	46.239	5.4		.871	1.00	54.69
ATOM		•	E1 GI	N 74	3	46.898	5.9		.051	1.00	57.62
			E2 GI	N 74:	3	46.202	5.1		. 749	1.00	59.09
ATOM		-	GI	N 743	3 .	47.816	7.2		.268	1.00	59.45
ATOM		_	GL			47.365	4.7		212	1.00	44.41
ATOM			AR			18.515	3.6		182	1.00	44.39
ATOM			AR			10.000	5.3		212	1.00	42.87
ATOM	5888	GB CB	AR			8.902	4.5	06 34.		_	41.45
ATOM	5889			_		9.350	5.39	97 32.			37.34
ATOM	5890	) CD			•	8.316	6.38	32.			
ATOM	5891	NE	ARC		-	8.854	7.20	7 31.			32.30
ATOM	5893	CZ	ARC			7.921	8.27	6 30.			31.37
ATOM	5894	NH				8.271	9.49	2 30.			36.76
ATOM	5897					9.553	9.81	3 30.3			39.88
ATOM	5900	С	ARG		4	7.330	10.40	4 30.3			39.94
ATOM	5901	0	ARG	·		0.068	3.61				9.12
ATOM	5902	N	PRO			0.813	3.94		0.5		1.40
MOTA	5903	CD	PRO			0.203	2.44				2.84
ATOM	5904	CA			49	345	1.739				0.11
ATOM	5905	CB	PRO	745	51	332	1.607				9.91
ATOM	5906	CG	PRO	745		.019	0.261				8.58
ATOM	5907	C	PRO	745	50	.250	0.645				7.46
ATOM	5908		PRO	745	52	.640	2.202			.00 3	7.41
ATOM	5909	0	PRO	745	52	.634	3.027				7.73
ATOM	5911	N	THR	746		. 753	1.843	34.37			7.71
	5912	CA	THR	746		. 050	2.328			00 35	5.90
	5913	CB	THR	746	56	. 085	2.380	33.91			.77
<b>-</b>		OG1	THR	746	56.	296	1.059	35.07	_		. 85
<b>-</b>	5915	CG2	THR	746	55.	605	2 202	35.60			. 92
	5916	C	THR	746		544	3.302	36.17		00 32	.17
	5917	0	THR	746		026	1.327	32.87	0 1.0		.69
3	5918	N	PHE	747		538	0.213	32.79			. 56
3	920	CA	PHE	747	57.		1.708	32.06			. 04
3.55.5	921	CB	PHE	747	58.	121	0.782	31.08		0 31	
	922	CG	PHE	747	50.	±21	1.472	30.19	3 1.0		
		CD1	PHE	747	57.		2.287	29.096			
ATOM 5		CD2	PHE	747	56.		1.666	28.092			
		CE1	PHE	747	57.		3.667	29.091			
<b>3</b>		CE2			56.:	L70	2.407	27.100		_	
		CZ		747	57.(	001	4.413	28.091			
			~ 1112	747	56.2	76	3.776	27.103		_	
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ATOM	5928	C	PHE	747	57.714	-0.413	31.782	1.00	31.92
MOTA	5929	0	PHE	747	57.727	-1.514	31.243	1.00	32.46
MOTA	5930	N	LYS	748	58.233	-0.199	32.986	1.00	33.47
MOTA	5932	CA	LYS	748	58.816	-1.302	33.733	1.00	35.57
MOTA	5933	CB	LYS	748	59.468	-0.800	35.026	1.00	39.42
ATOM	5934	CG	LYS	748	60.083	-1.923	35.861	1.00	46.49
MOTA	5935	CD	LYS	748	60.817	-1.407	37.103	1.00	50.69
MOTA	5936	CE	LYS	748	61.253	-2.574	37.999	1.00	52.57
ATOM	5937	NZ	LYS	748	62.072	-2.129	39.155	1.00	56.45
MOTA	5941	C	LYS	748	57.700	-2.318	34.028	1.00	35.58
ATOM	5942	0	LYS	748	57.898	-3.526	33.871	1.00	34.72
MOTA	5943	N	GLN	749	56.522	-1.818	34.411	1.00	35.59
ATOM	5945	CA	GLN	749	55.369	-2.684	34.692	1.00	38.20
ATOM	5946	CB	GLN	749	54.154	-1.872	35.162	1.00	42.73
ATOM	5947	CG	GLN	749	54.264	-1.171	36.499	1.00	49.30
ATOM	5948	CD	GLN	749	53.060	-0.282	36.761	1.00	53.13
MOTA	5949	OE1	GLN	749	53.194	0.915	37.023	1.00	52.71
MOTA	5950	NE2	GLN	749	51.873	-0.856	36.644	1.00	58.54
ATOM	5953	С	GLN	749	54.954	-3.392	33.409	1.00	36.16
ATOM	5954	0	GLN	749	54.745	-4.605	33.393	1.00	36.67
MOTA	5955	N	LEU	750	54.801	-2.609	32.342	1.00	35.83
MOTA	5957	CA	LEU	750	54.381	-3.117	31.037	1.00	34.49
ATOM	5958	CB	LEU	750	54.324	-1.988	30.004	1.00	32.49
MOTA	5959	CG	LEU	750	53.206	-0.958	30.188	1.00	31.94
MOTA	5960	CD1	LEU	750	53.411	0.230	29.267	1.00	30.45
MOTA	5961	CD2	LEU	750	51.859	-1.610	29.933	1.00	29.30
ATOM	5962	C	LEU	750	55.294	-4.214	30.559	1.00	33.87
ATOM	5963	0	LEU	750	54.828	-5.208	30.027	1.00	34.72
ATOM	5964	N	VAL	751	56.598	-4.038	30.759	1.00	36.12
ATOM	5966	CA	VAL	751	57.585	-5.045	30.363	1.00	34.50
ATOM	5967	CB	VAL	751	59.054	-4.532	30.559	1.00	31.96
ATOM	5968	CG1	VAL	751	60.052	-5.646	30.308	1.00	30.24
ATOM	5969	CG2	VAL	751	59.342	-3.386	29.604	1.00	28.02
MOTA	5970	С	VAL	751	57.349	-6.321	31.182	1.00	36.11
ATOM	5971	0	VAL	751	57.333	-7.422	30.638	1.00	36.45
ATOM	5972	N	GLU	752	57.107	-6.165	32.479	1.00	37.83
ATOM	5974	CA	GLU	752	56.869	-7.326	33.331	1.00	41.47
MOTA	5975	CB	GLU	752	56.800	-6.910	34.804	1.00	43.03
ATOM	5976	CG	GLU	752	58.122	-6.305	35.263	1.00	52.52
MOTA	5977	CD	GLU	752	58.251	-6.176	36.761	1.00	57.18
MOTA	5978	OE1	GLU	752	58.600	-5.068	37.233	1.00	58.11
MOTA	<b>597</b> 9	OE2	GLU	752	58.032	-7.191	37.461	1.00	61.59
ATOM	5980	C	GLU	752	55.623	-8.097	32.890	1.00	40.16
ATOM	5981	0	GLU	752	55.689	-9.308	32.642	1.00	39.75
ATOM	5982	N	ASP	753	54.524	-7.376	32.696	1.00	40.06
ATOM	5984	CA	ASP	753	53.275	-7.982	32.264	1.00	39.73
MOTA	5985	CB	ASP	753	52.157	-6.947	32.247	1.00	41.00
MOTA	5986	CG	ASP	753	51.668	-6.591	33.640	1.00	45.17
ATOM	5987	OD1	ASP	753	51.753	-7.468	34.543	1.00	49.78
MOTA	5988	OD2	ASP	753	51.210	-5.439	33.829	1.00	45.51
ATOM	5989	C	ASP	753	53.396	-8.595	30.890	1.00	39.64
ATOM	5990	0	ASP	753	52.955	-9.720	30.674	1.00	41.84
ATOM	5991	N	LEU	754	53.998	-7.861	29.960	1.00	37.75
MOTA	5993	CA	LEU	754	54.161	-8.358	28.603	1.00	38.16

Δ	TOM 5	004										
		994	CB	LEU	754	54.6	64	-7.2	261 27	664		_
		995	_	LEU	754	53.5		-6.2	•		1.0	
				LEU	754	54.1		-5.0		307	1.0	
				LEU	754	52.4		-6.9		590	1.0	
				LEU	754	55.0		-9.5			1.0	+
				LEU	754	54.9		~10.4			1.0	
			N )	ASP	755	56.0					1.0	
			CA 1	ASP	755	56.9		-9.6			1.00	
			CB p	SP	755	57.9		-10.7			1.00	40.87
AT		04 (	CG A	SP	755	59.12		-10.4			1.00	45.11
AT		05 (	DD1 A	SP	755	59.75		-11.4			1.00	48.64
AT		06 C	D2 A		755	59.43		-11.63			1.00	54.27
ATO		07 C			755			-11.95			1.00	
ATO	OM 60	08 0			755	56.08		-11.95	52 29.9	47	1.00	
ATO		09 N		_	756	56.15		-12.99		89	1.00	,
ATC		ll C	_		756	55.23		-11.77		55	1.00	
ATC	OM 60:		_		756	54.34		-12.81	7 31.4		1.00	
ATC	M 603					53.57		-12.31	6 32.6		1.00	40.24
ATO					756	52.43		-13.21	7 33.13		1.00	
ATO					756	51.79		-12.63	1 34.38		1.00	42.12
ATO					56	51.35	3	-11.24	7 34.18		1.00	42.33
ATO					56	50.295		-10.89	1 33.46		1.00	46.68
ATO					56	49.549	•	-11.818		6	1.00	48.17
ATO					56	49.998	}	-9.605			1.00	46.64
ATO	4 602	-	AR		56	53.362		-13.275			1.00	48.92
ATOM		-	AR		56	53.247	•	-14.469				40.19
ATON		_	IL:		57	52.688		12.327			1.00	42.24
ATOM					57	51.706	-	12.649			1.00	38.18
ATOM						50.952		11.382			1.00	38.40
ATOM						49.952		11.758			00	36.55
ATOM						50.216	-	10.726	29.364		00	34.67
ATOM				_	7	49.554		-9.423	29.048		.00	34.65
ATOM		_	ILE	_	7	52.301	_	13.400	27.500		.00	36.49
ATOM		_	ILE		7	51.709	_	14.360	27.025		.00	39.19
ATOM			VAL		8	53.492		12.996			.00	39.66
ATOM			VAL	75	8	54.161		13.645	27.061		.00	42.36
ATOM			VAL	75	8	55.582		13.052	25.937		.00	43.15
ATOM	6039	CG1		75	В	56.308		L3.855	25.682		.00	41.72
ATOM	6040	CG2	VAL	751	3	55.491		1.619	24.621			41.57
ATOM	6041	C	VAL	758	3	54.299		5.133	25.229			40.06
ATOM	6042	0	VAL	758	3	54.045	- 1	5.971	26.231			47.11
	6043	N	ALA	759	)	54.695	- 1	5.446	25.369			48.62
MOTA	6045	CA	ALA	759	<b>)</b>	54.879	1	6.820	27.464		00	49.64
ATOM	6046	CB	ALA	759	1	55.423	_ 1	6.020	27.908	1.	00	51.35
ATOM	6047	C	ALA	759		53.568		6.830	29.317	l.	00 9	50.11
ATOM	6048	0	ALA	759		53.520		7.598	27.850	l.		54.72
ATOM	6049	N	LEU	760		52.496		8.717	27.348	1.		58.64
ATOM	6051	CA	LEU	760				6.983	28.329	1.		54.84
ATOM	6052	CB	LEU	760		51.194		7.628	28.343	1.0		55.87
MOTA	6053	CG	LEU	760		50.330		7.034	29.459	1.0		6.85
ATOM	6054	CD1	LEU	760		50.875		7.165	30.885	1.0		6.80
ATOM	6055	CD2	LEU	760		49.991	-16	5.392	31.849	1.0		6.78
ATOM	6056	C	LEU	760		50.959		3.631	31.289	1.0		7.78
ATOM	6057	0	LEU			50.454		.546	27.013	1.0	-	7.36
ATOM	6058	N	THR	760		49.262		.859	26.944	1.0		7.65
			1117	761	!	51.151	-17		25.956	1.0		7.65 8.71
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ATOM	6060	CA	THR	761	50.541	-17.025	24.630	1.00	59.04	
MOTA	6061	CB	THR	761	50.839	-15.657	23.971	1.00	56.72	
ATOM	6062	OG1	THR	761	50.287	-14.610	24.775	1.00	56.53	
ATOM	6064	CG2	THR	761	50.213	-15.584	22.590	1.00	53.81	
MOTA	6065	C	THR	761	51.049	-18.138	23.721	1.00	60.44	
ATOM	6066	0	THR	761	52.255	-18.295	23.530	1.00	61.40	
MOTA	6067	SG	CYS	1603	18.474	-8.976	20.202	0.50	37.82	PRT2
ATOM	6068	CG	MET	534	69.311	12.109	23.281	0.50	36.25	PRT2
ATOM	6069	SD	MET	534	69.286	12.958	24.867	0.50	42.66	PRT2
ATOM	6070	CE	MET	534	70.539	12.083	25.804	0.50	43.27	PRT2
ATOM	6071	SG	CYS	603	56.046	-7.949	16.446	0.50	36.47	PRT2
MOTA	2676	OH2	TIP3	1	71.794	25.061	2.660	1.00	24.53	
MOTA	2679	OH2	TIP3	2	39.750	3.992	15.898	1.00	39.62	
MOTA	2682	OH2	TIP3	3	83.809	19.717	10.596	1.00	28.26	
ATOM	2685	OH2	TIP3	4	83.630	20.056	7.685	1.00	26.19	
ATOM	2688	OH2	TIP3	5	75.073	16.616	6.785	1.00	26.48	
MOTA	2691	OH2	TIP3	6	86.549	19.594	9.502	1.00	33.65	
ATOM	2694	OH2	TIP3	7	51.913	11.060	24.263	1.00	35.55	
ATOM	2697	OH2	TIP3	8	55.093	9.421	22.524	1.00	26.63	
ATOM	2700	OH2	TIP3	9	57.161	4.614	32.443	1.00	29.69	
MOTA	2703	OH2	TIP3	10	52.169	4.735	13.281	1.00	22.61	
ATOM	2706	OH2	TIP3	11	41.110	5.543	22.764	1.00	41.60	
MOTA	2709	OH2	TIP3	12	45.145	8.857	21.555	1.00	36.99	
ATOM	2712	OH2	TIP3	13	64.465	-2.607	28.883	1.00	30.17	
ATOM	2715	OH2	TIP3	14	76.944	13.287	23.954	1.00	32.94	
MOTA	2718	OH2	TIP3	15	79.062	17.048	18.200	1.00	51.65	
MOTA	2721	OH2	TIP3	16	83.066	11.657	15.958	1.00	25.12	
ATOM	2724	OH2	TIP3	17	13.957	-9.951	0.095	1.00	26.02	
MOTA	2727	OH2	TIP3	18	38.359	-0.001	5.000	1.00	37.43	
ATOM	2730	OH2	TIP3	19	5.442	2.705	19.077	1.00	29.46	
MOTA	2733	OH2	TIP3	20	27.008	6.166	4.885	1.00	25.05	
ATOM	2736	OH2	TIP3		34.242	-1.725	16.911	1.00	52.12	
ATOM	2739	OH2	TIP3		20.167	2.428	27.681	1.00	42.69	
ATOM	2742	OH2		23	50.794	-11.834	38.045	1.00	60.16	
ATOM	2745	OH2		24	17.261	-5.993	-1.757	1.00	25.88	
ATOM	2748	OH2	TIP3		27.516	7.803	15.070	1.00	39.33	
ATOM	2751	OH2	TIP3		31.574	0.146	6.684	1.00	35.78	
ATOM	2754	OH2	TIP3		27.119	-12.972	27.844	1.00	43.66	
ATOM	2757	OH2	TIP3		28.439	-17.074	13.203	1.00	36.44	
MOTA	2760	OH2	TIP3		88.706	14.393	7.969	1.00	32.49	
ATOM	2763	OH2	TIP3		-2.338	-3.424	11.295	1.00	49.20	
ATOM	2766	OH2	TIP3		35.086	-4.130	18.836	1.00	37.83	
ATOM	2769	OH2	TIP3	32	80.455	17.922	9.507	1.00	23.69	
ATOM	2772	OH2		33	5.538	3.619	10.835		29.13	
ATOM	2775	OH2	TIP3		-10.685	5.290	11.288	1.00	24.40	
ATOM	2778	OH2	TIP3		29.210	-8.799	20.241	1.00	46.52	
MOTA	2781	OH2	TIP3		6.195	3.150	13.803	1.00	31.39	
ATOM	2784	OH2	TIP3		31.898	2.830	0.154	1.00	40.17	
ATOM	2787	OH2	TIP3		19.915	2.023	-3.939	1.00	31.34	
ATOM	2790	OH2	TIP3		62.242	2.604	32.859	1.00	39.67	
ATOM	2793	OH2	TIP3		21.231	-7.063	-3.900	1.00	23.55	
ATOM	2796	OH2	TIP3		-15.809	8.838	22.610	1.00	36.02	
ATOM	2799	OH2	TIP3		40.120	2.154	8.433	1.00	60.62	
ATOM	2802	OH2	TIP3	43	19.583	11.128	-0.045	1.00	37.85	



ATC			2 TI	23 44	67.05	6 9.03	17700		
ATC			2 TI	3 45					
ATC			2 TIF	3 46					
ATC		4 OH	2 TIP	3 47					
ATO				3 48	66.48				
ATO			2 TIP	3 49	85.00			_	
ATO			2 TIP	3 50	-4.57				
ATO			2 TIP	3 51	19.49		_ · · <u>_</u>		
ATO			TIP.	3 52	67.49			1.00	
ATO			TIP:	3 53	34.79			1.00	
ATO			TIP:	3 54	34.787			1.00	40.16
ATO			TIP	3 55	59.972			1.00	39.46
ATON			TIPS	3 56	-7.139		27.870	1.00	31.56
ATON			TIPE	3 57	54.998		6.345 25.360	1.00	42.00
MOTA			TIPE	58	68.697		16.740	1.00	42.05
ATOM			TIP3	59	73.750		19.041	1.00	46.12
ATOM			TIP3	60	3.431			1.00	32.26
ATOM			TIP3	61	37.904		-8.218 5.612	1.00	31.22
ATOM			TIP3	62	29.982		-1.303	1.00	33.72
ATOM			TIP3	63	66.918		8.678	1.00	39.11
ATOM			TIP3	64	49.117	1.310	12.227	1.00	34.68
ATOM			TIP3	65	41.246	3.987	29.033	1.00	34.31
ATOM			TIP3	<b>6</b> 6	10.755	-12.957	1.167	1.00	34.55
ATOM			TIP3	67	-1.184	-4.327	21.439	1.00	42.14
ATOM	2877		TIP3	68	30.349	16.267	13.265	1.00	37.90
ATOM	2880	OH2	TIP3	69	8.111	4.362	3.445	1.00 1.00	55.23
ATOM ATOM	2883	OH2	TIP3	70	73.131	18.780	22.628	1.00	23.88
ATOM	2886	OH2	TIP3	71	-7.949	-3.409	24.953	1.00	40.20
ATOM	2889	OH2	TIP3	72	66.379	-4.621	28.423	1.00	35.49 45.46
ATOM	2892	OH2	TIP3	73	21.506	-20.711	4.815	1.00	52.46
ATOM	2895 2898	OH2	TIP3	74	59.539	~6.865	4.928	1.00	48.87
ATOM	2901	OH2 OH2	TIP3	75	16.565	-13.297	-3.008	1.00	51.80
ATOM	2904	OH2	TIP3	76	-15.235	7.385	4.428	1.00	29.13
ATOM	2907	OH2	TIP3	77	32.926	2.785	13.213	1.00	37.62
ATOM	2910	OH2	TIP3 TIP3	78	0.246	-2.768	10.996	1.00	28.25
ATOM	2913	OH2		79	17.495	2.354	5.447	1.00	23.63
ATOM	2916	OH2		80 81	6.336	2.434	21.950	1.00	29.56
ATOM	2919	OH2		82	27.374	3.628	6.163	1.00	34.06
ATOM	2922	OH2	TIP3		-8.708	6.263	9.522	1.00	30.34
ATOM	2925	OH2	TIP3		1.500	-1.935		1.00	27.61
ATOM	2928	OH2		85	-4.825	-3.133		1.00	33.50
ATOM	2931	OH2	TIP3		17.513	2.839			24.27
ATOM	2934	OH2		87	20.298	3.414		1.00	26.15
ATOM	2937	OH2		88	0.488			1.00	25.95
MOTA	2940	OH2		89	19.939	-6.185		1.00	19.14
ATOM	2943			90	10.670	-15.654		1.00	33.36
ATOM	2946			91	4.107			1.00	33.92
ATOM	2949			92	6.238			1.00	23.31
ATOM	2952			93	-13.563	1.438			27.86
ATOM	2955			94	15.707	-7.454			26.69
ATOM	2958		TIP3 9		-1.856 12.654	-5.393		.00	9.91
ATOM	2961			6	69.774	4.928			31.32
	2964		TIP3 9			27.363			5.86
		_		•	24.636	-13.192	0.040 1	.00 4	8.53
CCC									

MOTA	2967	OH2	TIP3 98	60.453	-4.625	33.829	1.00	31.97
ATOM	2970	OH2	TIP3 99	10.513	5.719	3.487	1.00	38.90
ATOM	2973	OH2	TIP3 10		-4.011	4.342	1.00	30.61
ATOM	2976	OH2	TIP3 10:		-1.608	10.514	1.00	36.08
ATOM	2979	OH2	TIP3 102		5.709	30.608	1.00	29.38
ATOM	2982	OH2	TIP3 10:		0.702	11.792	1.00	47.80
ATOM	2985	OH2	TIP3 104		6.325	16.924	1.00	24.03
ATOM	2988	OH2	TIP3 109		0.656	19.432	1.00	53.74
MOTA	2991	OH2	TIP3 106	5.620	-8.417	22.266	1.00	51. <b>9</b> 0
ATOM	2994	OH2	TIP3 10'		8.294	17.464	1.00	35.23
ATOM	2997	OH2	TIP3 108		-10.556	-1.042	1.00	27.83
ATOM	3000	OH2	TIP3 109		1.846	18.172	1.00	30.90
MOTA	3003	OH2	TIP3 110		12.643	3.558	1.00	33.82
MOTA	3006	OH2	TIP3 111		13.617	33.196	1.00	54.79
ATOM	3009	OH2	TIP3 112	_	-10.740	1.991	1.00	37.96
ATOM	3012	OH2	TIP3 113		2.913	0.958	1.00	29.64
ATOM	3015	OH2	TIP3 114		1.753	25.812	1.00	38.73
ATOM	3018	OH2	TIP3 115		15.535	14.189	1.00	35.24
ATOM	3021	OH2	TIP3 116		-11.312	9.146	1.00	32.85
ATOM	3024	OH2	TIP3 117		26.360	12.964	1.00	41.83
MOTA	3027	OH2	TIP3 118		-6.579	-3.252	1.00	42.78
ATOM	3030	OH2	TIP3 119		4.493	4.305	1.00	28.32
ATOM	3033	OH2	TIP3 120		-13.690	8.639	1.00	33.73
ATOM	3036	OH2	TIP3 121		6.329	10.373	1.00	31.72
ATOM	3039	OH2	TIP3 122		3.686	15.591	1.00	32.37
ATOM	3042	OH2	TIP3 123		3.790	20.450	1.00	35.80
ATOM	3045	OH2	TIP3 124		-11.467	22.590	1.00	45.12
ATOM	3048	OH2	TIP3 125		2.412	16.576	1.00	41.90
ATOM ATOM	3051	OH2	TIP3 126		-11.905	7.083	1.00	24.83
ATOM	3054 3057	OH2 OH2	TIP3 127		3.860	-1.622	1.00	35.46
ATOM	3060	OH2	TIP3 128 TIP3 129		5.755	12.352	1.00	35.43
ATOM	3063	OH2	TIP3 129 TIP3 130		6.932	2.982	1.00	40.68
ATOM	3066	OH2	TIP3 130		-1.778	0.201	1.00	34.99
ATOM	3069	OH2	TIP3 131		10.362	11.064	1.00	42.31
ATOM	3072	OH2	TIP3 133	· · · · ·	-12.638	18.958	1.00	58.71
ATOM	3075	OH2	TIP3 133	57.560	11.540 -10.846	21.428	1.00	36.75
ATOM	3078	OH2	TIP3 135		15.001	14.099 16.515	1.00	52.90
ATOM	3081	OH2	TIP3 136	85.717	11.251		1.00	37.81
ATOM	3084	OH2	TIP3 137	12.951	-2.469	2.075	1.00	35.18 22.07
ATOM	3087	OH2	TIP3 138		3.486		1.00	38.01
ATOM	3090	OH2	TIP3 139		7.412	-2.649	1.00	33.50
ATOM	3093	OH2	TIP3 140		-9.970	0.974	1.00	26.14
ATOM	3096	OH2	TIP3 141	59.480	10.772	14.098	1.00	52.08
ATOM	3099	OH2	TIP3 142	13.869	-16.121	3.919	1.00	40.06
ATOM	3102	OH2	TIP3 143	-6.407	-3.413	16.641	1.00	44.38
ATOM	3105	OH2	TIP3 144	25.667	-12.645	3.411	1.00	48.28
ATOM	3108	OH2	TIP3 145	-16.282	10.641	6.423	1.00	40.94
MOTA	3111	OH2	TIP3 146	86.637	12.861	7.008	1.00	39.45
ATOM	3114	OH2	TIP3 147	32.082	-4.569	1.892	1.00	27.35
ATOM	3117	OH2	TIP3 148	44.809	7.627	11.670	1.00	35.65
MOTA	3120	OH2	TIP3 149	80.693	12.459	16.523	1.00	37.21
MOTA	3123	OH2	TIP3 150	2.941	-7.118		1.00	38.43
ATOM	3126	OH2	TIP3 151	31.794	-6.086	20.704	1.00	42.80



ATO	_		12 T	IP3 15	2	74.77	0 -2.6	02 20 0		
ATO		32 OH	12 T	IP3 15		7.73	_			0 40.40
ATC	DM 31:	35 ОН		P3 15		71.61				0 35.61
ATC	DM 313	38 OH		P3 15		68.113				0 40.14
ATC				P3 15				-		0 34.38
ATO	M 314	4 OH		P3 15		0.042				33.08
ATO				P3 15		68.020			95 1.00	
ATO	M 315			P3 15		3.795				
ATO	M 315					52.106		_		40.06
ATO	M 315					6.414			9 1.00	
ATO	M 315					-10.282				
ATO	M 316					76.410			1 1.00	
ATON	M 316					9.910	-12.04		7 1.00	32.79
ATON						33.983	14.21		1 1.00	
ATOM						2.330	-7.95	2 16.978		
ATOM						29.701	1.78		7 1.00	
ATOM						32.494	-17.319	9 11.798		
ATOM						42.107	17.932			44.83
ATOM						87.822	10.537	7 5.568		54.30
ATOM				_		70.261	-4.143	25.064		44.75
ATOM				_		77.519	5.882	23.891		42.67
ATOM			TIP			-0.921	-8.166	4.521		45.91
ATOM			TIP			34.213	15.329			40.10
ATOM			TIP			-9.647	7.731			
ATOM			TIP			11.619	5.799			35.63 36.36
ATOM	3201		TIP:			-8.709	13.964			51.97
ATOM	3207	OH2	TIP			31.770	3.376			
ATOM	3210	OH2	TIP			-8.494	9.789	24.269		46.26 50.98
ATOM	3213	OH2		3 179		-1.234	-6.253	15.622	1.00	38.47
ATOM	3216	OH2		180		80.252	0.887	15.691	1.00	39.48
ATOM	3219	OH2	TIPS			67.248	20.272	-1.555	1.00	
ATOM	3222		TIP3			-0.566	4.367	1.362	1.00	48.22
ATOM	3225	OH2	TIP3	_		0.120	6.523	2.615	1.00	39.84
ATOM	3228	OH2	TIP3			-1.496	8.789	1.237	1.00	33.11
ATOM	3231	OH2	TIP3			-5.143	9.130	2.236	1.00	41.03
ATOM	3234	OH2	TIP3		-	-7.275	10.106	3.833	1.00	40.47
ATOM	3234	OH2	TIP3			2.717	7.275	0.769	1.00	40.55
ATOM	3237	OH2	TIP3	188		5.176	10.645	8.459	1.00	44.67
ATOM	3243	OH2	TIP3	189	6	3.822	12.690	22.883	1.00	34.48
ATOM	3246	OH2	TIP3	190	7	9.109	1.028	18.201	1.00	41.88
ATOM		OH2	TIP3		5	9.332	-11.681	7.236	1.00	46.40
ATOM	3249	OH2	TIP3	192		3.967	-1.218	-4.268	1.00	63,45
ATOM	3252	OH2	TIP3	193	5	9.444	2.867	33.368		34.79
ATOM	3255	OH2	TIP3	194		2.024	13.487	19.852		41.00
ATOM	3258	OH2	TIP3	195		2.101	16.218	22.802		53.61
ATOM	3261	OH2	TIP3	196		0.987	-8.546	14.474		44.03
	3264	OH2	TIP3	197	_	0.491	5.461		_	41.38
ATOM	3267	OH2	TIP3	198		1.179	6.795	30.372		38.51
ATOM	3270	OH2	TIP3	199	-:	1.365	-4.128	11.905		41.77
ATOM	3273	OH2	TIP3	200	8:	1.440	15.558	27.656		50.98
ATOM	3276	OH2		201		7.491	4.116	17.262	_	44.47
ATOM	3279	OH2		202		7.546	10.513	23.873		50.58
MOTA	3282			203		1.992	4.513	14.499		39.06
	3285	OH2		204		3.486	4.513 -4.591	27.719		19.89
MOTA	3288	OH2		205		2.799		9.171		19.53
						,	7.848	22.320	1.00 4	13.50

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ATOM	3291	OH2	TIP3 20	6 52.728	11.884	21.811	1.00	39.98
ATOM		OH2	TIP3 20	7 26.706	14.069	19.833	1.00	46.68
ATOM	3297	OH2	TIP3 20	8 -7.154	8.907	6.444	1.00	42.83
ATOM	3300	OH2	TIP3 20	9 86.648	5.606	16.034	1.00	51.15
ATOM	3303	OH2	TIP3 21	0 54.879	15.840	20.379	1.00	50.23
ATOM	3306	OH2	TIP3 21	1 51.417	19.473	22.691	1.00	48.35
ATOM	3309	OH2	TIP3 21	2 20.102	6.924	7.085	1.00	38.15
MOTA	3312	OH2	TIP3 21	3 28.991	1.941	-3.570	1.00	47.39
ATOM	3315	OH2	TIP3 21	4 26.505	2.386	-4.633	1.00	46.48
ATOM	3318	OH2	TIP3 21	5 36.482	2.810	18.521	1.00	46.26
ATOM	3321	OH2	TIP3 21	6 16.941	-20.504	14.128	1.00	49.74
ATOM	3324	OH2	TIP3 21	7 28.572	-14.448	6.157	1.00	49.13
MOTA	3327	OH2	TIP3 21	8 31.380	1.471	-1.998	1.00	43.02
MOTA	3330	OH2	TIP3 21	9 10.065	-16.338	15.455	1.00	42.75
ATOM	3333	OH2	TIP3 22	0 7.350	-11.974	5.652	1.00	55.35
ATOM	3336	OH2	TIP3 22	1 -12.328	14.547	10.986	1.00	51.29
ATOM	3339	OH2	TIP3 22:	2 11.186	9.609	-1.388	1.00	37.68
ATOM	3342	OH2	TIP3 22	3 11.389	12.276	-1.400	1.00	46.93
ATOM	3345	OH2	TIP3 224		13.069	-1.161	1.00	41.79
ATOM	3348	OH2	TIP3 22	5 31.303	17.822	7.853	1.00	48.21
ATOM	3351	OH2	TIP3 22	36.875	11.804	-2.106	1.00	59.03
ATOM	3354	OH2	TIP3 22		3.048	11.020	1.00	50.41
ATOM	3357	OH2	TIP3 228	63.950	13.409	26.627	1.00	43.40
ATOM	3360	OH2	TIP3 225	36.367	6.116	15.221	1.00	57.79
ATOM	3363	OH2	TIP3 230		4.355	6.342	1.00	47.53
MOTA	3366	OH2	TIP3 23	50.038	-11.673	10.767	1.00	56.90
MOTA	3369	OH2	TIP3 232	60.196	-10.144	16.590	1.00	51.61
MOTA	3372	OH2	TIP3 23	18.021	-21.179	7.008	1.00	49.93
ATOM	3375	OH2	TIP3 234	66.236	-1.218	30.583	1.00	39.55
ATOM	3378	OH2	TIP3 23!	74.959	18.928	20.659	1.00	38.04
ATOM	3381	OH2	TIP3 236	-2.816	10.082	3.187	1.00	49.31
ATOM	3384	OH2	TIP3 23	5.894	-3.410	25.289	1.00	35.55
MOTA	3387	OH2	TIP3 238	35.784	6.047	12.543	1.00	41.96
ATOM	3390	OH2	TIP3 239	-5.400	16.537	14.180	1.00	43.13
MOTA	3393	OH2	TIP3 240	46.589	-11.622	26.970	1.00	43.71
MOTA	3396	OH2	TIP3 241	6.199	6.592	13.797	1.00	46.51
MOTA	3399	OH2	TIP3 242	-3.777	-5.158	20.907	1.00	42.08
MOTA	3402	OH2	TIP3 243	1.969	-3.711	-0.282	1.00	37.38
MOTA	3405	OH2	TIP3 244	86.200	11.629	22.877	1.00	56.51
MOTA	3408	OH2	TIP3 249		7.565	5.514	1.00	47.58
MOTA	3411	OH2	TIP3 246	4.802	8.149	2.136	1.00	50.70
MOTA	3414	OH2	TIP3 247	64.590	-8.128	20.596	1.00	43.65
ATOM	3417	OH2	TIP3 248		-17.840	13.283	1.00	47.64
ATOM	3420	OH2	TIP3 249	42.116	-6.808	14.953	1.00	53.79
MOTA	3423	OH2	TIP3 250	2.745	-4.054	22.128	1.00	60.88
MOTA	3426	OH2	TIP3 251	71.999	1.177	-2.124	1.00	47.90
ATOM	3429	OH2	TIP3 252	50.328	-3.210	33.068	1.00	57.01
MOTA	3435	OH2	TIP3 253		9.337	11.631	1.00	52.55
MOTA	3438	OH2	TIP3 254	43.373	20.489	30.490	1.00	51.97
MOTA	3441	OH2	TIP3 255	67.045	16.529	15.793	1.00	49.02
ATOM	3444	OH2	TIP3 256	87.509	21.566	5.114	1.00	54.21
MOTA	3447	OH2	TIP3 257	21.060	10.052	-9.215	1.00	60.32
ATOM	3450	OH2	TIP3 258	11.827	2.450	27.951	1.00	54.26
MOTA	3453	OH2	TIP3 259	64.788	-0.418	3.563	1.00	50.94
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ATOM ATOM ATOM ATOM ATOM ATOM	3456 3459 3462 3465 3468 3471	OH2 OH2 OH2 OH2 OH2 OH2	TIP3 TIP3 TIP3 TIP3 TIP3	261 262 263 264	25.605 -18.804 30.652 22.350	28.473 -8.106 10.886 11.349 -16.098	16.201 -2.742	1.00 1.00 1.00 1.00	62.81 52.81 55.25 50.40 53.27
ATOM	34/1	OH2	TIP3	265	29.720	9.106	18.465	1.00	57.23

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## TABLE 2

Atom		Atom	A.A	A.A	x	Y	z	occ	В	
No.		Туре	Type	No.						
ATOM	1	N	GLU	1464	-13.425	16.769	8.973	1.00	61.21	
MOTA	3	CA	GLU	1464	-12.536	16.852	7.821	1.00	59.70	
MOTA	4	CB	GLU	1464	-11.383	17.829	8.085	1.00	60.05	
MOTA	5	С	GLU	1464	-11.998	15.478	7.427	1.00	57.11	
ATOM	6	0	GLU	1464	-12.134	15.076	6.274	1.00	59.75	
MOTA	7	N	LEU	1465	-11.406	14.749	8.368	1.00	52.21	
MOTA	9	CA	LEU	1465	-10.871	13.424	8.062	1.00	46.72	
MOTA	10	CB	LEU	1465	-10.102	12.844	9.249	1.00	44.98	
MOTA	11	CG	LEU	1465	-8.608	13.123	9.384	1.00	46.11	
MOTA	12	CD1	LEU	1465	-8.338	14.592	9.663	1.00	51.13	
MOTA	13	CD2	LEU	1465	-8.064	12.286	10.512	1.00	4.99	
MOTA	14	C	LEU	1465	-12.000	12.475	7.700	1.00	44.16	
ATOM	15	0	LEU	1465	-13.101	12.577	8.239	1.00	44.04	
ATOM	16	N	PRO	1466	-11.760	11.580	6.732	1.00	42.53	
ATOM	17	CD	PRO	1466	-10.535	11.534	5.913	1.00	41.30	
MOTA	18	CA	PRO	1466	-12.740	10.591	6.269	1.00	41.16	
ATOM	19	CB	PRO	1466	-12.134	10.111	4.959	1.00	41.48	
MOTA	20	CG	PRO	1466	-10.658	10.213	5.220	1.00	41.30	
ATOM	21	С	PRO	1466	-12.906	9.441	7.261	1.00	41.31	
ATOM	22	0	PRO	1466	-11.929	8.936	7.816	1.00	41.05	
ATOM	23	N	GLU	1467	-14.145	9.044	7.500	1.00	41.02	
ATOM	25	CA	GLU	1467	-14.428	7.960	8.427	1.00	42.42	
ATOM	26	CB	GLU	1467	-15.931	7.904	8.712	1.00	47.98	
ATOM	27	CG	GLU	1467	-16.565	9.238	9.105	1.00	52.79	
ATOM	28	CD	GLU	1467	-17.998	9.093	9.606	1.00	54.21	
ATOM	29	OE1	GLU	1467	-18.474	7.949	9.741	1.00	58.90	
ATOM	30	OE2	GLU	1467	-18.650	10.120	9.879	1.00	55.90	
ATOM	31	c	GLU	1467	-13.972	6.628	7.837	1.00	40.93	
ATOM	32	Ö	GLU	1467	-14.061	6.426	6.620	1.00	44.32	
ATOM	33	N	ASP	1468	-13.473	5.731	8.689	1.00	35.10	
MOTA	35	CA	ASP	1468	-13.024	4.404	8.256	1.00	31.82	
MOTA	36	CB	ASP	1468	-11.507	4.358	7.992	1.00	30.65	
ATOM	37	CG	ASP	1468	-11.025	3.002	7.440	1.00	29.93	
ATOM	38	OD1	ASP	1468	-11.689	1.958	7.603	1.00	29.63	
ATOM	39	OD2	ASP	1468	-9.945	2.974	6.835	1.00	33.63	
ATOM	40	c	ASP	1468	-13.394	3.441	9.369	1.00	31.81	
ATOM	41	ō	ASP	1468	-12.618	3.209	10.302	1.00	31.91	
ATOM	42	N	PRO	1469	-14.569	2.819	9.247	1.00	29.68	
ATOM	43	CD	PRO	1469	-15.482	2.963	8.097	1.00	28.33	
ATOM	44	CA	PRO	1469	-15.100	1.863	10.220	1.00	31.80	
ATOM	45	CB	PRO	1469	-16.352	1.331	9.510	1.00	32.51	
MOTA	46	CG	PRO	1469	-16.332	2.496	8.656	1.00	27.41	
ATOM	47	C	PRO	1469	-14.146	0.731	10.590	1.00	30.44	
MOTA	48	0	PRO	1469	-14.140	0.731	11.654	1.00		
ATOM	49	N	ARG	1470	-14.272	0.133	9.704	1.00	30.02 31.06	
ATOM	51	CA	ARG	1470	-13.196	-0.636	9.704	1.00		
MOTA	52	CB	ARG	1470	-12.240	-0.860	8.660	1.00	31.86	
ATOM									31.36	
ATOM	53	CG	ARG	1470	-12.107	-1.437	7.448	1.00	33.08	

A:	TOM 5	4 C	D AR	G 1470		_			
A:	rom 5	5 N	E AR	•				8 1.00	31.08
A	rom 5	7 C		_	-0.54			1 1.00	
	TOM 58	_	H1 AR	•	05			9 1.00	33.32
ΑΊ	OM 61		H2 ARC		20	_		5 1.00	
ΤA	OM 64		ARC		-9.15	,		7 1.00	
AT	'OM 65		ARC		-11.29				
AT	OM 66	N	TRE		-10.820	_		3 1.00	33.43
AT	OM 68	CA			-11.031			1.00	31.84
AT	OM 69	CB			-10.063			1.00	31.17
AT	OM 70	CG			-8.816			1.00	30.15
ATO	-	CD		· <del>-</del>	-8.173			1.00	29.54
ATO		CE			-7.288			1.00	31.07
ATO	DM 73	CE		1471	-6.913			1.00	34.41
ATC	OM 74	CD		1471	-6.762	-0.768		1.00	29.46
ATC		NE:		1471	-8.309	0.660		1.00	30.20
ATO	M 77	CZ		1471	-7.557	-0.371		1.00	33.09
ATO	M 78	CZ		1471	-6.042	-2.085	10.135	1.00	31.68
ATO	M 79	CH2		1471	-5.897	-1.853	12.540	1.00	29.65
ATO.	M 80	C	TRP	1471	-5.541	-2.494	11.347	1.00	30.18
ATO	M 81	0	TRP	1471	-10.477	2.019	13.620	1.00	29.94
ATO	M 82	N	GLU	1472	-9.782	2.108	14.631	1.00	30.00
ATO	M 84	CA	GLU	1472	-11.573	2.737	13.416	1.00	29.06
ATON	M 85	CB	GLU	1472	-12.051	3.706	14.380	1.00	28.62
ATON		CG	GLU	1472	-13.312	4.386	13.849	1.00	29.16
ATOM		CD	GLU	1472	-13.641	5.733	14.529	1.00	30.74
ATOM		OE1	GLU	1472	-12.676 -12.090	6.848	14.156	1.00.	30.05
ATOM		OE2	GLU		-12.511	6.799	13.057	1.00	31.32
ATOM		С	GLU		-12.327	7.784	14.961	1.00	30.26
ATOM		. 0	GLU		-12.969	3.159	15.767	1.00	28.70
ATOM		N	LEU		-11.810	2.125	15.916		31.01
ATOM		CA	LEU		-12.054	3.842	16.781		27.38
ATOM		CB	LEU		-10.763	3.451	18.161	1.00	29.61
ATOM		CG	LEU		-10.923	3.073	18.899	1.00	28.56
ATOM		CD1	LEU		-11.485	2.756	20.403	1.00	30.06
ATOM	98	CD2	LEU	1473	~9.595	1.354 2.876	20.639	1.00	28.42
ATOM	99	C	LEU	1473 -	12.617	4.714	21.115		28.15
ATOM	100	0			12.179	5.814	18.764		31.81
ATOM	101	N	PRO		13.670	4.591	18.407		3.00
ATOM	102	CD	PRO		14.488	3.400			1.45
ATOM	103	CA	PRO :		14.261				1.72
ATOM	104	CB	PRO :		15.400	_		1.00 3	1.23
ATOM	105	CG	PRO 1		15.815				9.01
ATOM	106	C	PRO 1	L474 -	13.217				9.09
ATOM	107	0	PRO 1		12.447				3.36
ATOM	108	N	ARG 1		13.188				6.40
ATOM	110	CA	ARG 1		12.228				3.67
ATOM	111			_	12.433				3.96
ATOM	112	CG		-	12.134				5.31
ATOM	113				2.060		_		0.10
ATOM	114				1.785				2.98
ATOM	116					4.0			. 91
ATOM	117								.30
ATOM	120	NH2	ARG 1				_		.88
				_		-4.30/ 1	6.943 1	.00 40	. 98

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ATOM	123	С	ARG	1475	-12.278	8.142	23.404	1.00	35.88
ATOM	124	0	ARG	1475	-11.240	8.046	24.061	1.00	37.10
MOTA	125	N	ASP	1476	-13.479	7.920	23.928	1.00	36.47
ATOM	127	CA	ASP	1476	-13.632	7.581	25.335	1.00	37.24
ATOM	128	CB	ASP	1476	-15.112	7.629	25.741	1.00	39.66
MOTA	129	CG	ASP	1476	-15.930	6.480	25.163	1.00	42.38
ATOM	130	OD1	ASP	1476	-15.438	5.706	24.322	1.00	47.52
ATOM	131	OD2	ASP	1476	-17.098	6.349	25.568	1.00	48.06
ATOM	132	C	ASP	1476	-13.023	6.232	25.724	1.00	36.93
ATOM	133	0	ASP	1476	-13.034	5.856	26.898	1.00	40.09
MOTA	134	N	ARG	1477	-12.564	5.475	24.732	1.00	34.34
ATOM	136	CA	ARG	1477	-11.961	4.171	24.993	1.00	32.47
ATOM	137	CB	ARG	1477	-12.269	3.212	23.852	1.00	31.59
ATOM	138	CG	ARG	1477	-13.716	2.939	23.640	1.00	29.66
ATOM	139	CD	ARG	1477	-14.314	2.342	24.875	1.00	30.65
ATOM	140	NE	ARG	1477	-14.498	3.342	25.918	1.00	31.37
ATOM	142	CZ	ARG	1477	-14.822	3.055	27.174	1.00	32.81
ATOM	143	NHl	ARG	1477	-15.002	1.794	27.549	1.00	33.92
ATOM	146	NH2	ARG	1477	-14.950	4.025	28.062	1.00	31.74
ATOM	149	С	ARG	1477	-10.452	4.266	25.153	1.00	33.13
ATOM	150	0	ARG	1477		3.281	25.445	1.00	33.55
ATOM	151	N	LEU	1478	-9.923	5.466	24.984	1.00	34.43
ATOM	153	CA	LEU	1478	-8.493	5.663	25.076	1.00	35.68
MOTA	154	CB	LEU	1478	-8.008	6.350	23.790	1.00	34.98
ATOM	155	CG	LEU	1478	-6.581	6.137	23.284	1.00	31.11
ATOM	156	CD1	LEU	1478	-6.280	4.650	23.161	1.00	26.62
ATOM	157	CD2	LEU	1478	-6.428	6.839	21.940	1.00	28.80
ATOM	158	С	LEU	1478	-8.158	6.505	26.295	1.00	36.21
MOTA	159	0	LEU	1478	-8.501	7.688	26.361	1.00	39.67
ATOM	160	N	VAL	1479	-7.558	5.878	27.293	1.00	35.42
MOTA	162	CA	VAL	1479	-7.156	6.599	28.491	1.00	35.80
ATOM	163	CB	VAL	1479	-7.269	5.707	29.742	1.00	36.29
ATOM	164	CG1	VAL	1479	-7.017	6.527	30.983	1.00	37.23
ATOM	165	CG2	VAL	1479	-8.650	5.059	29.812	1.00	34.41
ATOM	166	С	VAL	1479	-5.704	7.046	28.244	1.00	35.68
ATOM	167	0	VAL	1479	-4.764	6.246	28.319	1.00	33.45
MOTA	168	N	LEU	1480	-5.538	8.315	27.885	1.00	38.15
MOTA	170	CA	LEU	1480	-4.213	8.860	27.584	1.00	42.61
MOTA	171	CB	LEU	1480	-4.332	10.205	26.857	1.00	39.14
ATOM	172	CG	LEU	1480	-4.969	10.179	25.460	1.00	38.44
MOTA	173	CD1	LEU	1480	-4.901	11.579	24.879	1.00	39.39
ATOM	174	CD2	LEU	1480	-4.263	9.194	24.533	1.00	36.86
ATOM	175	С	LEU	1480	-3.274	8.970	28.783	1.00	46.37
ATOM	176	0	LEU	1480	-3.659	9.445	29.850	1.00	48.86
MOTA	177	N	GLY	1481	-2.033	8.537	28.594	1.00	47.13
MOTA	179	CA	GLY	1481	-1.081	8.573	29.678	1.00	48.19
ATOM	180	С	GLY	1481	0.163	9.388	29.425	1.00	50.27
MOTA	181	0	GLY	1481	0.152	10.367	28.675	1.00	51.19
ATOM	182	N	LYS	1482	1.240	8.965	30.078	1.00	50.93
ATOM	184	CA	LYS	1482	2.543	9.606	30.007	1.00	50.94
MOTA	185	CB	LYS	1482	3.509	8.866	30.933	1.00	50.41
MOTA	186	CG	LYS	1482	4.971	9.026	30.567	1.00	51.87
ATOM	187	CD	LYS	1482	5.810	7.874	31.087	1.00	53.49
ATOM	188	CE	LYS	1482	5.390	6.542	30.478	1.00	50.77

			NZ	LYS	1482	6.25	1 c	422				
	_		C :	LYS	1482				. 986	1.00		2
			0 1	LYS	1482	- · <b>-</b> ·	_		609	1.00	52.31	L
			N I	PRO	1483				851	1.00		
			CD I	PRO	1483	3.667			250	1.00	53.47	
	_		CA E	PRO	1483	00			997	1.00	54.19	
	OM 19	-	CB F	RO	1483	4.772			937	1.00	54.10	ı
AT			G p	RO	1483	3.772	_		976	1.00		
AT			. P	RO	1483	5.535			895	1.00	55.30	
ATO			P	RO	1483	6.343				1.00	54.72	
AT(	_ •		L	EU	1484	5.619	_			1.00	53.48	
ATO		_	A L		1484	6.739	· <del>-</del>			1.00	57.05	
ATC			B L		1484	6.307	8.4			1.00	59.26	
ATC					1484	5.391	7.2			1.00	59.35	
ATC					1484	4.975	6.2			1.00	60.87	
ATO	•		02 LE		1484	6.081	5.16			1.00	57.14	
ATO		•	LE	: บ	1484	7.847	5.57			1.00	59.79	
ATO		•	LE	U :	L484	8.980	9.19 8.72			1.00	61.30	
ATO		•	GL	Y 1	485	7.494	10.35			1.00	62.17	
ATO			GL	Y 1	485	8.456	11.17			1.00	63.75	
ATO		_	GL	Y 1	485	8.081	11.17			1.00	66.33	
IOTA IOTA		•	${ t GL}$	Y 1	485	6.918	11.65			1.00	67.79	
ATO			GL	N 1	491	4.615	13.76	_		1.00	69.61	
ATOM		•••			491	4.353	13.35			1.00	58.26	
ATOM		CB	GLI	_	491	3.476	14.37			1.00	57.98	
ATOM		CG	GLi		491	3.134	14.034			1.00	61.80	
ATOM		CD	GL		491	2.019	14.91			1.00	70.31	
ATOM		OE:		_	491	1.355	15.636			1.00	75.91	
ATOM		NE2			191	1.820	14.832		_	1.00	77.85	
ATOM		C	GLN		191	3.709	11.965		_	.00	78.30	
ATOM		O N	GLN		191	2.701	11.669		_		54.67	
ATOM	230	N CA	VAL		92	4.305	11.125				54.91	
ATOM	231	CB	VAL		92	3.825	9.763	20.98			50.04	
ATOM	232	CG1	VAL		92	4.861	8.705	20.58			44.93	
ATOM	233	CG2	VAL		92	4.378	7.325	20.958			42.65	
ATOM	234	C	VAL	14		5.119	8.766	19.09			39.71	
ATOM	235	0	VAL	14		3.584	9.661	22.490			40.98	
ATOM	236	N	VAL VAL	14		4.451	10.029	23.289			43.43 13.43	
ATOM	238	CA	VAL	14		2.400	9.212	22.888			11.13	
MOTA	239	CB	VAL	14		2.107	9.080	24.304		_	88.77	
MOTA	240	CG1	VAL	14:		1.052	10.133	24.782			6.35	
ATOM	241	CG2	VAL	149		1.410	11.508	24.287			6.06	
ATOM	242	C	VAL			-0.329	9.755	24.339			7.64	
ATOM	243	0	VAL	149		1.589	7.693	24.619			7.77	
ATOM	244	N	LEU	149		0.948	7.058	23.783			8.88	
ATOM	246	CA	LEU	149		1.949	7.187	25.790		_	6.24	
ATOM	247	CB	LEU	149		1.468	5.880	26.205	1.		5.92	
ATOM	248	CG	LEU	149		2.252	5.383	27.429	1.6		5.41	
ATOM	249	CD1	LEU	149		1.886	4.009	28.004	1.0		5.21	
ATOM	250	CD2	LEU	149		1.927	2.931	26.924	1.0		3.60	
ATOM	251	C	LEU	149		2.835	3.670	29.145	1.0		5.03	
ATOM	252	0	LEU	149 149		0.010	6.095	26.564	1.0		5.27	
ATOM	253	N	ALA	149		0.425	7.215	26.887	1.0		.35	
				±33	<i>-</i>	0.807	5.043	26.468	1.0		. 93	
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ATOM	255	CA	ALA	1495	-2.220	5.145	26.768	1.00	34.44
MOTA	256	CB	ALA	1495	-2.955	5.794	25.616	1.00	35.29
MOTA	25.7	С	ALA	1495	-2.781	3.770	27.018	1.00	34.59
MOTA	258	0	ALA	1495	-2.128	2.766	26.748	1.00	35.52
MOTA	259	N	GLU	1496	-3.996	3.723	27.536	1.00	36.64
ATOM	261	CA	GLU	1496	-4.652	2.462	27.806	1.00	37.57
ATOM	262	CB	GLU	1496	-5.000	2.354	29.287	1.00	38.97
MOTA	263	CG	GLU	1496	-3.769	2.304	30.185	1.00	41.79
MOTA	264	CD	GLU	1496	-4.110	2.475	31.645	1.00	43.65
ATOM	265	OE1	GLU	1496	-4.408	3.617	32.036	1.00	42.97
ATOM	266	OE2	GLU	1496	-4.086	1.475	32.398	1.00	46.65
ATOM	267	С	GLU	1496	-5.896	2.404	26.943	1.00	38.50
ATOM	268	0	GLU	1496	-6.660	3.371	26.867	1.00	40.28
ATOM	269	N	ALA	1497	-6.051	1.301	26.223	1.00	37.34
ATOM	271	CA	ALA	1497	-7.194	1.131	25.352	1.00	37.42
MOTA	272	CB	ALA	1497	-6.743	0.625	23.985	1.00	35.92
ATOM	273	С	ALA	1497	-8.146	0.148	26.000	1.00	36.77
ATOM	274	0	ALA	1497	-7.759	-0.977	26.323	1.00	35.74
ATOM	275	N	ILE	1498	-9.354	0.616	26.291	1.00	37.03
ATOM	277	CA	ILE	1498	-10.378	-0.224	26.896	1.00	36.80
ATOM	278	СВ	ILE	1498	-11.372	0.612	27.728	1.00	34.53
ATOM	279	CG2	ILE	1498	-12.373	-0.290	28.425	1.00	34.59
ATOM	280	CG1	ILE	1498	-10.640	1.438	28.778	1.00	31.97
ATOM	281	CD1	ILE	1498	-11.552	2.344	29.541	1.00	31.12
ATOM	282	C	ILE	1498	-11.126	-0.807	25.709	1.00	38.72
ATOM	283	o	ILE	1498	-11.647	-0.066	24.879	1.00	37.74
MOTA	284	N	GLY	1499	-11.137	-2.126	25.590	1.00	40.98
ATOM	286	CA	GLY	1499	-11.839	-2.728	24.482	1.00	44.64
ATOM	287	C.	GLY	1499	-10.931	-3.115	23.332	1.00	48.45
ATOM	288	0	GLY	1499	-10.260	-4.147	23.401	1.00	51.92
ATOM	289	N	LEU	1500	-10.877	-2.269	22.303	1.00	47.87
ATOM	291	CA	LEU	1500	-10.076	-2.530	21.102	1.00	46.80
ATOM	292	СВ	LEU	1500	-8.594	-2.770	21.434	1.00	45.37
ATOM	293	CG	LEU	1500	-7.543	-1.661	21.293	1.00	44.84
ATOM	294	CD1	LEU	1500	-6.174	-2.290	21.450	1.00	43.33
ATOM	295	CD2	LEU	1500	-7.623	-0.959	19.948	1.00	40.43
ATOM	296	C	LEU	1500	-10.631	-3.737	20.349	1.00	45.63
ATOM	297	0	LEU	1500	-10.797	-4.823	20.915	1.00	44.42
ATOM	298	N	PRO	1505	-13.569	-5.910	25.549	1.00	52.13
ATOM	299	CD	PRO	1505	-14.316	-7.170	25.398	1.00	54.09
ATOM	300	CA	PRO	1505	-14.451	-4.828	25.999	1.00	50.46
ATOM	301	CB	PRO	1505	-15.841	-5.455	25.891	1.00	49.86
ATOM	302	CG	PRO	1505	-15.586	-6.898	26.193	1.00	52.17
ATOM	303	c	PRO	1505	-14.136	-4.370	27.422	1.00	47.75
ATOM	304	ō	PRO	1505	-14.148	-3.180	27.710	1.00	47.93
ATOM	305	N	ASN	1506	-13.778	-5.313	28.285	1.00	46.20
ATOM	307	CA	ASN	1506	-13.778	-4.986	29.666	1.00	49.52
ATOM	308	CB	ASN			-5.829	30.612	1.00	
ATOM	308	CG		1506 1506	-14.310 -15.788			1.00	52.42
			ASN	1506		-5.489	30.526		54.50
ATOM	310	OD1	ASN	1506	-16.179	-4.331 -6.480	30.680	1.00	57.16
ATOM	311	ND2	ASN	1506	-16.610	-6.489	30.244	1.00	56.82
MOTA	314	C	ASN	1506	-11.973	-5.124	30.003	1.00	50.65
ATOM	315	0	ASN	1506	-11.583	-5.174	31.178	1.00	50.65
ATOM	316	N	ARG	1507	-11.142	-5.145	28.968	1.00	50.90



							200			
ΑT	MOT	318	CA	A	RG 150	17 0 7				
	MOT	319	CB		RG 150			· <b>-</b>		49.77
		320	CG		RG 150					
		321	CD		RG 150					
		322	NE		RG 150					
AT	OM	324	cz		RG 150	0.00			83 1.00	72.55
AT	OM .	325	NH1						94 1.00	
AT	OM :	328	NH2						92 1.00	
ATO	OM :	331	C	AR		9.55				79.30
ATO		332	0	AR	•					45.60
ATO	OM 3	333	N	VA	•.					42.08
ATC		335	CA	VA						42.86
ATC	M 3	36	CB	VA					8 1.00	40.75
ATC	M 3	37	CG1	VA		50.			0 1.00	38.75
ATO	м з	38	CG2	VA			_		2 1.00	43.29
ATO		39	C	VAI					2 1.00	37.56
ATO	М 3	40	0	VAI		-5.929				39.14
ATO	М 3	41	N	THE		-5.369			8 1.00	39.16
ATO	_	43	CA	THE		-5.517			7 1.00	37.26
ATO		44	CB	THE		-4.298	_		5 1.00	36.52
ATO		45	OG1	THR		-4.571			1.00	37.83
ATON	1 34	17	CG2	THR		-5.423	-4.340		1.00	43.88
ATON		18	C	THR	1509	-3.267	-3.540		1.00	34.51
ATOM		19	0	THR		-3.434	-1.495		1.00	35.82
ATOM	1 35		N	LYS		-3.927	-0.408	_		34.37
ATOM		2	CA	LYS	1510	-2.175	-1.628		1.00	35.96
ATOM		3	CB	LYS	1510	-1.291	-0.479		1.00	36.13
ATOM			CG	LYS	1510	-0.032 -0.277	-0.695			37.77
MOTA	35	5 (	CD	LYS	1510	1.023	-0.854		1.00	44.58
ATOM	35	6 (	CE	LYS	1510	0.947	-0.658	29.948	1.00	51.33
ATOM	35	7 1	JZ	LYS	1510	-0.149	-1.286	31.342	1.00	58.15
ATOM	36:		2	LYS	1510	-0.929	-0.728	32.187	1.00	64.94
ATOM	362		)	LYS	1510	-0.574	-0.355	25.373		34.59
ATOM	363		J	VAL	1511	-1.092	-1.345	24.734	1.00	31.43
ATOM	365		'A	VAL	1511	-0.810	0.846	24.835		32.95
ATOM	366		B '	VAL	1511	-2.129	1.121	23.441	1.00	32.29
ATOM	367	_	Gl '	VAL	1511	-2.879	1.213	22.621	1.00	32.95
ATOM	368	_	G2 1	VAL	1511	-3.026	-0.109 2.354	22.686	1.00	34.79
ATOM	369	_	7	VAL	1511	-0.058		23.148	1.00 3	32.84
ATOM	370	-	7	VAL	1511	0.021	2.446 3.185	23.353		2.65
ATOM	371		•	<b>ALA</b>	1512	0.521	2.721	24.344		1.62
ATOM	373	C	A A	ALA.	1512	1.244	3.969	22.186		0.24
ATOM	374	CI	3 A	LA	1512	2.599	3.700	21.954		8.18
ATOM	375	C	A	LA	1512	0.373	4.783	21.316	1.00 2	5.62
ATOM	376	0	A	LA	1512	-0.151		21.015	1.00 2	7.54
ATOM	377	N	v	ΆL	1513	0.204	4.264	20.040	1.00 2	7.17
MOTA	379	CA	v	AL	1513	-0.630	6.054	21.322	1.00 3	0.52
ATOM	380	CE	V.	AL	1513	-1.731	6.914	20.503	1.00 3	4.08
ATOM	381	CG	1 v.	AL	1513	-2.607	7.591	21.347	1.00 34	1.61
ATOM	382	CG			1513	-2.567	8.444	20.474		5.75
ATOM	383	C			1513	0.203	6.549	22.087		3.45
ATOM	384	0			1513	0.203	8.008	19.837	_	3.38
ATOM	385	N			1514	0.105		20.510		3.32
ATOM	387	CA			1514	0.818		18.513		.19
					- <b>-</b>	0.010	9.104	17.746		.12
CCCD/FF.										

ATOM	388	CB	LYS	1514	1.339	8.513	16.439	1.00	40.93
ATOM	389	CG	LYS	1514	2.452	7.488	16.632	1.00	42.52
MOTA	390	CD	LYS	1514	2.861	6.803	15.338	1.00	46.25
ATOM	391	CE	LYS	1514	3.268	7.796	14.261	1.00	49.76
MOTA	392	NZ	LYS	1514	4.304	8.771	14.705	1.00	52.14
ATOM	396	С	LYS	1514	-0.166	10.215	17.458	1.00	40.69
ATOM	397	0	LYS	1514	-1.313	9.953	17.110	1.00	41.69
ATOM	398	N	MET	1515	0.277	11.454	17.613	1.00	43.28
ATOM	400	CA	MET	1515	-0.569	12.610	17.379	1.00	46.21
ATOM	401	CB	MET	1515	-1.363	12.936	18.644	1.00	46.96
ATOM	402	CG	MET	1515	-0.488	13.293	19.837	1.00	47.61
ATOM	403	SD	MET	1515	-1.413	13.464	21.358	1.00	49.77
ATOM	404	CE	MET	1515	-1.593	11.761	21.814	1.00	47.84
MOTA	405	С	MET	1515	0.299	13.805	17.000	1.00	49.90
ATOM	406	0	MET	1515	1.519	13.788	17.194	1.00	49.83
MOTA	407	N	LEU	1516	-0.339	14.822	16.430	1.00	54.45
ATOM	409	CA	LEU	1516	0.335	16.053	16.023	1.00	57.57
MOTA	410	СВ	LEU	1516	-0.483	16.762	14.944	1.00	54.10
ATOM	411	CG	LEU	1516	-0.800	16.007	13.664	1.00	50.71
ATOM	412	CD1	LEU	1516	-1.830	16.800	12.901	1.00	51.20
ATOM	413	CD2	LEU	1516	0.467	15.809	12.849	1.00	50.08
ATOM	414	С	LEU	1516	0.487	17.010	17.202	1.00	61.88
ATOM	415	0	LEU	1516	-0.170	16.852	18.235	1.00	63.30
MOTA	416	N	LYS	1517	1.335	18.018	17.021	1.00	66.83
ATOM	418	CA	LYS	1517	1.568	19.036	18.037	1.00	71.46
MOTA	419	СВ	LYS	1517	2.985	19.593	17.911	1.00	76.28
ATOM	420	CG	LYS	1517	4.084	18.626	18.349	1.00	82.19
ATOM	421	CD	LYS	1517	5.450	19.085	17.846	1.00	86.93
ATOM	422	CE	LYS	1517	6.579	18.228	18.411	1.00	90.46
MOTA	423	NZ	LYS	1517	7.896	18.513	17.763	1.00	92.51
MOTA	427	C	LYS	1517	0.549	20.156	17.837	1.00	72.44
MOTA	428	0	LYS	1517	-0.142	20.198	16.819	1.00	72.12
MOTA	429	N	SER	1518	0.474	21.075	18.793	1.00	73.90
ATOM	431	CA	SER	1518	-0.470	22.185	18.697	1.00	74.96
ATOM	432	CB	SER	1518	-0.498	22.980	20.002	1.00	74.72
ATOM	433	С	SER	1518	-0.133	23.100	17.525	1.00	76.16
ATOM	434	0	SER	1518	-1.029	23.667	16.897	1.00	76.56
ATOM	435	N	ASP	1519	1.158	23.245	17.232	1.00	77.24
MOTA	437	CA	ASP	1519	1.601	24.094	16.125	1.00	78.51
ATOM	438	CB	ASP	1519	2.849	24.888	16.535	1.00	79.70
MOTA	439	C	ASP	1519	1.887	23.264	14.865	1.00	78.29
MOTA	440	0	ASP	1519	2.797	23.580	14.088	1.00	78.52
MOTA	441	N	ALA	1520	1.121	22.192	14.682	1.00	76.90
MOTA	443	CA	ALA	1520	1.285	21.313	13.529	1.00	74.09
MOTA	444	CB	ALA	1520	0.737	19.930	13.840	1.00	74.20
MOTA	445	С	ALA	1520	0.580	21.895	12.318	1.00	71.82
ATOM	446	0	ALA	1520	-0.573	22.311	12.400	1.00	71.78
MOTA	447	N	THR	1521	1.291	21.951	11.202	1.00	69.97
MOTA	449	CA	THR	1521	0.734	22.480	9.970	1.00	68.86
MOTA	450	СВ	THR	1521	1.848	22.911	9.026	1.00	68.87
ATOM	451	OG1	THR	1521	2.621	21.762	8.651	1.00	70.03
ATOM	453	CG2	THR	1521	2.756	23.912	9.715	1.00	71.55
MOTA	454	C	THR	1521	-0.081	21.389	9.292	1.00	67.89
ATOM	455	0	THR	1521	0.111	20.204	9.563	1.00	69.03
•		-			J				05



ATO			GL	J 1522	-0.964	21.78	3 8.38	2 1 00	
ATO				J 1522				_	
ATO.			GL	J 1522	-2.737				- · · -
ATO			GLU	1522	-0.886				
ATO		0	GLU	1522	-1.324				
ATO		N	LYS	1523	0.367	20.205			
ATO		CA	LYS	1523	1.314	19.326			
ATO		CB	LYS		2.629	20.064			
ATON		CG	LYS		3.815	19.162		•	
ATON	467	CD	LYS		3.510				
ATOM	468	CE	LYS		4.759	18.288			
MOTA	1 469	NZ	LYS		4.429	17.596			65.88
ATOM	1 473	C	LYS		1.565	16.721			70.37
ATOM	474	0	LYS	1523		18.173	6.974		54.80
ATOM	475	N	ASP	1524	1.548	17.003	6.581		54.44
ATOM	477	CA	ASP	1524	1.786	18.523	8.239		51.67
ATOM	478	CB	ASP	1524	2.036	17.549	9.295	1.00	49.43
ATOM	479	CG	ASP	1524	2.297	18.271	10.622	1.00	51.06
MOTA	480	OD1	ASP	1524	3.598	19.080	10.613	1.00	54.03
ATOM		OD2	ASP		3.649	20.136	11.283	1.00	56.32
ATOM		C	ASP	1524 1524	4.580	18.658	9.956	1.00	56.02
ATOM	483	Ó	ASP		0.847	16.596	9.413	1.00	47.73
ATOM	484	N	LEU	1524	1.017	15.387	9.580	1.00	45.85
ATOM	486	CA	LEU	1525	-0.354	17.155	9.300	1.00	47.62
ATOM	487	CB	LEU	1525	-1.585	16.380	9.354	1.00	45.95
ATOM	488	CG	LEU	1525	-2.801	17.307	9.271	1.00	43.61
ATOM	489	CD1		1525	-4.193	16.665	9.234	1.00	44.56
ATOM	490	CD2	LEU	1525	-4.364	15.543	10.268	1.00	46.02
ATOM	491	C C	LEU	1525	-5.215	17.740	9.468	1.00	43.80
ATOM	492	0	LEU	1525	~1.605	15.372	8.210	1.00	45.67
ATOM	493	N	LEU	1525	-1.921	14.204	8.416	1.00	46.78
ATOM	495		SER	1526	-1.245	15.822	7.014	1.00	45.44
ATOM	496	CA CB	SER	1526	-1.211	14.945	5.851	1.00	46.33
ATOM	497	OG	SER	1526	-0.903	15.744	4.584	1.00	48.48
ATOM	499	C	SER	1526	-2.012	16.546	4.218	1.00	57.28
ATOM	500	0	SER	1526	-0.192	13.821	5.995	1.00	43.84
ATOM	501		SER	1526	-0.480	12.669	5.674	1.00	45.24
ATOM	503	N	ASP	1527	0.994	14.144	6.489	1.00	40.88
ATOM		CA	ASP	1527	2.024	13.128	6.646	1.00	39.70
ATOM	504 505	CB	ASP	1527	3.376	13.767		1.00	37.62
ATOM		CG	ASP	1527	3.934	14.555	5.786		37.01
ATOM	506 507	OD1	ASP	1527	3.399	14.434	4.657	1.00	35.78
ATOM		OD2	ASP	1527	4.916	15.295	5.992	1.00	40.23
ATOM	508	C	ASP	1527	1.652	12.053	7.659	1.00	38.51
	509	0	ASP	1527	1.951	10.872	7.461	1.00	37.68
ATOM	510	N	LEU	1528	0.973	12.460	8.725		
ATOM	512	CA	LEU	1528	0.532	11.513	9.744		38.16
ATOM	513	CB	LEU	1528	0.026	12.258	10.985		38.29
ATOM	514	CG	LEU	1528	-0.505	11.412	12.153		37.12
MOTA	515	CD1	LEU	1528	0.499	10.323	12.539		39.03
ATOM	516	CD2	LEU	1528	-0.825	12.315	13.334		35.39
ATOM	517	C	LEU	1528	-0.568	10.611			35.29
ATOM	518	0		1528	-0.607	9.400			38.10
ATOM	519	N		1529	-1.450	11.210			37.21
ATOM	521	CA		1529	-2.531	10.472			36.71
				-	1	10.4/2	7.718	1.00	35.93

ATOM	522	CB	ILE	1529	-3.486	11.419	6.931	1.00	35.67	
ATOM	523	CG2	ILE	1529	-4.492	10.619	6.119	1.00	34.04	
ATOM	524	CG1	ILE	1529	-4.259	12.295	7.916	1.00	33.81	
MOTA	525	CD1	ILE	1529	-5.177	13.288	7.276	1.00	33.58	
ATOM	526	C	ILE	1529	-1.912	9.447	6.786	1.00	37.49	
ATOM	527	0	ILE	1529	-2.274	8.269	6.829	1.00	37.11	
ATOM	528	N	SER	1530	-0.926	9.893	6.003	1.00	38.20	
ATOM	530	CA	SER	1530	-0.217	9.036	5.050	1.00	37.49	
ATOM	531	CB	SER	1530	0.911	9.822	4.370	1.00	43.32	
ATOM	532	OG	SER	1530	0.424	10.970	3.687	1.00	52.31	
ATOM	534	С	SER	1530	0.382	7.808	5.719	1.00	34.40	
ATOM	535	0	SER	1530	0.234	6.691	5.219	1.00	31.51	
ATOM	536	N	GLU	1531	1.048	8.028	6.851	1.00	32.08	
ATOM	538	CA	GLU	1531	1.690	6.952	7.594	1.00	30.60	
ATOM	539	CB	GLU	1531	2.506	7.515	8.759	1.00	29.70	
ATOM	540	CG	GLU	1531	3.094	6.428	9.657	1.00	30.53	
ATOM	541	CD	GLU	1531	3.871	6.962	10.839	1.00	33.17	
MOTA	542	OE1	GLU	1531	4.473	6.134	11.552	1.00	33.38	
MOTA	543	OE2	GLU	1531	3.883	8.193	11.062	1.00	37.52	
ATOM	544	C	GLU	1531	0.698	5.911	8.094	1.00	30.17	
ATOM	545	0	GLU	1531	0.991	4.714	8.100	1.00	29.76	
ATOM	546	N	MET	1532	-0.464	6.379	8.530	1.00	31.34	
MOTA	548	CA	MET	1532	-1.521	5.496	9.015	1.00	30.72	
ATOM	549	CB	MET	1532	-2.666	6.336	9.591	1.00	29.99	
ATOM	550	CG	MET	1532	-3.880	5.523	10.020	1.00	30.10	
ATOM	551	SD	MET	1532	-5.173	6.510	10.727	1.00	29.46	
ATOM	552	CE	MET	1532	-5.462	7.682	9.455	1.00	23.76	
MOTA	553	C	MET	1532	-2.025	4.638	7.843	1.00	30.47	
ATOM	554	0	MET	1532	-2.080	3.401	7.925	1.00	27.05	
ATOM	555	N	GLU	1533	-2.387	5.319	6.756	1.00	30.56	
ATOM	557	CA	GLU	1533	-2.863	4.674	5.542	1.00	30.56	
ATOM	558	CB	GLU	1533	-3.090	5.725	4.458	1.00	28.60	
ATOM	559	CG	GLU	1533	-4.226	6.677	4.761	1.00	29.08	
ATOM	560	CD	GLU	1533	-5.531	5.954	5.014	1.00	31.28	
ATOM	561	OE1	GLU	1533	-6.006	5.230	4.117	1.00	33.09	
ATOM	562	OE2	GLU	1533	-6.086	6.104	6.121	1.00	34.97	
ATOM	563	С	GLU	1533	-1.861	3.638	5.064	1.00	29.86	
ATOM	564	0	GLU	1533	-2.232	2.541	4.677	1.00	32.28	
ATOM	565	Ŋ	MET	1534	-0.590	4.014	5.107	1.00	32.54	
MOTA	567	CA	MET	1534	0.515	3.145	4.719	1.00	33.39	
MOTA	568	CB	MET	1534	1.826	3.894	4.885	1.00	34.70	
ATOM	569	CG	MET	1534	3.038	3.047	4.654	1.00	44.51	
ATOM	570	SD	MET	1534	3.479	3.063	2.943	1.00	52.81	
ATOM	571	CE	MET	1534	4.349	4.607	2.874	1.00	47.34	
ATOM	572	C	MET	1534	0.530	1.896	5.607	1.00	32.98	
ATOM	573	0	MET	1534	0.689	0.776	5.115	1.00	34.00	
ATOM	574	N	MET	1535	0.364	2.100	6.910	1.00	31.92	
ATOM	576	CA	MET	1535	0.336	0.986	7.848	1.00	30.80	
ATOM	577	CB	MET	1535	0.252	1.503	9.294	1.00	33.77	
ATOM	578	CG	MET	1535	1.509	2.216	9.810	1.00	32.26	
ATOM	579	SD	MET	1535	1.520	2.433	11.617	1.00	34.75	
ATOM	580	CE	MET	1535	1.183	4.173	11.723	1.00	37.86	
ATOM	581	С	MET	1535	-0.837	0.052	7.521	1.00	30.80	
ATOM	582	0	MET	1535	-0.704	-1.175	7.589	1.00	32.03	



ATO	M 583	N	LY						
			LI	S 1536	-1.97	4 0.63	8 7 34		
ATO			LY	S 1536	-3.17				
ATO	•		LY	S 1536	-4.33				
OTA			LY	S 1536	-4.86				
ATO		CD	LY	S 1536	-5.97				
ATO		CE	LY	S 1536	-6.43				
ATON		NZ	LY:		-7.57				
ATOM	1 594	C	LYS		-2.88				
MOTA	1 595	0	LYS		-3.23				
ATOM	596	N	MET		-2.30		_		
ATOM	598	CA	MET		-1.96				
ATOM	599	CB	MET		-1.37				31.53
ATOM	600	CG	MET		-2.377				35.11
ATOM	601	SD	MET						42.40
ATOM		CE	MET		-3.657				50.10
ATOM		C	MET		-3.069			1.00	50.20
ATOM	604	ō	MET		-0.976			1.00	30.86
ATOM	605	N	ILE		-1.218			1.00	30.07
ATOM	607	CA	ILE		0.119			1.00	30.92
ATOM	608	CB	ILE	1538	1.173		4.563	1.00	28.12
ATOM	609	CG2	ILE	1538	2.359		5.313	1.00	28.71
ATOM	610	CG1	ILE	1538	3.310	-3.303	5.865	1.00	29.72
ATOM	611	CD1		1538	3.126	-1.343	4.350	1.00	30.79
ATOM	612	CDI	ILE	1538	4.375	-0.745	4.945	1.00	32.46
ATOM	613	0	ILE	1538	0.717	-4.179	5.299	1.00	26.33
ATOM	614	N	ILE	1538	1.178	-5.276	4.996	1.00	24.20
ATOM	616	CA	GLY	1539	-0.188	-4.027	6.258	1.00	27.41
ATOM	617	CA	GLY	1539	-0.651	-5.190	6.997	1.00	27.83
ATOM	618	0	GLY	1539	0.240	-5.533	8.179	1.00	29.10
ATOM	619		GLY	1539	1.308	-4.937	8.368	1.00	30.33
ATOM	621	N	LYS	1540	-0.157	-6.561	8.916	1.00	29.46
ATOM	622	CA	LYS	1540	0.539	-6.976	10.120	1.00	29.27
ATOM		СВ	LYS	1540	-0.470	-7.520	11.139	1.00	27.01
ATOM	623	CG	LYS	1540	-1.438	-6.483	11.638	1.00	29.58
ATOM	624	CD	LYS	1540	-2.496	-7.103	12.530	1.00	39.41
ATOM	625	CE	LYS	1540	-3.548	-6.069	12.952	1.00	44.14
ATOM	626	NZ	LYS	1540	-2.994	-4.996	13.828	1.00	46.92
ATOM	630	C	LYS	1540	1.679	-7.962	10.020	1.00	27.17
ATOM	631	0	LYS	1540	1.745	-8.794	9.111	1.00	26.20
ATOM	632	N	HIS	1541	2.565	-7.856	11.006	1.00	26.20
	634	CA	HIS	1541	3.690	-8.761	11.144	1.00	
ATOM	635	CB	HIS	1541	4.787	-8.506	10.120	1.00	27.30
ATOM	636	CG	HIS	1541	5.849	-9.555	10.125		22.20
ATOM	637	CD2	HIS	1541	5.886	-10.789	9.555		21.32
ATOM	638	ND1	HIS	1541	7.052	-9.413	10.791		23.29
ATOM	640	CE1	HIS	1541	7.775	-10.509			19.41
ATOM	641	NE2	HIS	1541	7.097	-11.355			23.61
MOTA	643	C	HIS	1541	4.245	-8.640	9.889		21.81
ATOM	644	0	HIS	1541	4.290	7.549	12.565		28.64
ATOM	645	N	LYS	1542	4.650	-9.791	13.132		30.64
ATOM	647	CA	LYS	1542	5.200		13.108		29.47
ATOM	648	CB	LYS	1542	5.683	~9.893			28.78
ATOM	649		LYS	1542	6.232	-11.326			30.16
ATOM	650			1542	5.277	-11.572			32.63
	651			1542		-11.046			12.90
				<b>-</b> J74	5.659	-11.475	18.551		8.13

ATOM	652	NZ	LYS	1542	4.726	-10.930	19.564	1.00	54.87
ATOM	656	С	LYS	1542	6.351	-8.928	14.705	1.00	26.54
ATOM	657	0	LYS	1542	6.440	-8.321	15.773	1.00	26.19
ATOM	658	N	ASN	1543	7.193	-8.733	13.697	1.00	24.36
ATOM	660	CA	ASN	1543	8.357	-7.874	13.852	1.00	24.08
ATOM	661	CB	ASN	1543	9.601	-8.596	13.359	1.00	22.69
ATOM	662	CG	ASN	1543	9.781	-9.950	14.029	1.00	22.81
ATOM	663	OD1	ASN	1543	9.664	-10.996	13.388	1.00	23.62
MOTA	664	ND2	ASN	1543	10.028	-9.938	15.324	1.00	24.94
ATOM	667	С	ASN	1543	8.318	-6.429	13.377	1.00	23.48
ATOM	668	0	ASN	1543	9.351	-5.861	13.059	1.00	22.94
MOTA	669	N	ILE	1544	7.130	-5.821	13.380	1.00	24.15
MOTA	671	CA	ILE	1544	6.976	-4.407	13.012	1.00	24.60
ATOM	672	CB	ILE	1544	6.516	-4.191	11.531	1.00	24.90
MOTA	673	CG2	ILE	1544	7.495	-4.852	10.571	1.00	21.57
MOTA	674	CG1	ILE	1544	5.081	-4.688	11.316	1.00	26.66
MOTA	675	CD1	ILE	1544	4.481	-4.321	9.945	1.00	23.98
MOTA	676	C	ILE	1544	5.954	-3.785	13.955	1.00	24.78
MOTA	677	0	ILE	1544	5.160	-4.503	14.558	1.00	27.87
MOTA	678	N	ILE	1545	6.035	-2.474	14.159	1.00	26.39
MOTA	680	CA	ILE	1545	5.089	-1.779	15.025	1.00	26.79
MOTA	681	CB	ILE	1545	5.588	-0.345	15.384	1.00	28.85
ATOM	682	CG2	ILE	1545	4.512	0.449	16.103	1.00	23.60
MOTA	683	CG1	ILE	1545	6.833	-0.423	16.269	1.00	27.20
ATOM	684	CD1	ILE	1545	6.565	-0.990	17.639	1.00	27.12
MOTA	685	С	ILE	1545	3.792	-1.708	14.224	1.00	26.99
ATOM	686	0	ILE	1545	3.720	-1.023	13.197	1.00	27.61
ATOM	687	N	ASN	1546	2.809	-2.495	14.654	1.00	26.70
ATOM	689	CA	ASN	1546	1.514	-2.565	13.983	1.00	26.53
ATOM	690	СВ	ASN	1546	0.871	-3.953	14.169	1.00	26.23
ATOM	691	CG	ASN	1546	1.695	-5.072	13.551	1.00	24.96
MOTA	692	OD1	ASN	1546	1.773	-5.206	12.330	1.00	28.08
ATOM	693	ND2	ASN	1546	2.319	-5.872	14.387	1.00	22.38
ATOM	696	, C	ASN	1546	0.521	-1.497	14.418	1.00	26.89
ATOM	697	0	ASN	1546	0.610	-0.952	15.523	1.00	27.40
ATOM	698	N	LEU	1547	-0.349	-1.138	13.481	1.00	27.77
ATOM	700	CA	LEU	1547	-1.416	-0.175	13.701	1.00	28.28
ATOM	701	CB	LEU	1547	-1.958	0.313	12.361	1.00	27.04
MOTA	702	CG	LEU	1547	-3.199	1.194	12.408	1.00	25.74
ATOM	703	CD1	LEU	1547	-2.836	2.575	12.950	1.00	27.66
ATOM	704	CD2	LEU	1547	-3.799	1.289	11.014	1.00	23.38
ATOM	705	C	LEU	1547	-2.498	-0.972	14.435	1.00	29.80
ATOM	706	0	LEU	1547	-2.766	-2.135	14.105	1.00	28.63
ATOM	707	N	LEU	1548	-3.088	-0.351	15.448	1.00	29.91
ATOM	709	CA	LEU	1548	-4.114	-0.997	16.256	1.00	28.46
ATOM	710	CB	LEU	1548	-3.735	-0.956	17.749	1.00	26.76
ATOM	711	CG	LEU	1548	-2.460	-1.701	18.162	1.00	22.44
ATOM	712	CD1	LEU	1548	-2.277	-1.554	19.653	1.00	21.91
ATOM	713	CD2	LEU	1548	-2.551	-3.179	17.778	1.00	20.79
MOTA	714	C	LEU	1548	-5.480	~0.365	16.058	1.00	27.31
ATOM	715	0	LEU	1548	-6.489	-1.043	16.193	1.00	28.25
ATOM	716	N .	GLY	1549	-5.506	0.925	15.732	1.00	24.02
ATOM	718	CA	GLY	1549	-6.774	1.598	15.553	1.00	24.57
ATOM	719	С	GLY	1549	-6.548	3.077	15.395	1.00	25.19

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ATOM	720	0	GLY	1540	5	_			
ATOM	721	N	ALA		-5.400	3.488			
ATOM	723	CA	ALA		-7.617	3.875	15.427		
ATOM	724		ALA		-7.487	5.319	15.282		
ATOM	725	C	ALA		-7.206	5.680	13.824		24.29
ATOM	726	o	ALA	1550	-8.695	6.103	15.765		23.95
ATOM	727	N	CYS	1551	-9.810 -8.444	5.590	15.780		24.95
MOTA	729	CA	CYS	1551	-9.482	7.336	16.199		25.03
ATOM	730	CB	CYS	1551	-9.221	8.270	16.639		28.21
ATOM	731	SG	CYS	1551	-9.378	8.774	18.055	1.00	26.76
ATOM	732	С	CYS	1551	-9.359	7.521 9.426	19.317	1.00	34.39
ATOM	733	0	CYS	1551	-8.482		15.656	1.00	29.98
ATOM	734	N.	THR	1552	-10.198	10.281	15.800		32.14
ATOM	736	CA	THR	1552	-10.135	9.412 10.435	14.625	1.00	31.09
ATOM	737	CB	THR	1552	-10.052	9.781	13.595	1.00	32.91
ATOM	738	OG1	THR	1552	-11.276	9.097	12.189	1.00	32.60
ATOM	740	CG2	THR	1552	-8.928	8.768	11.890 12.144	1.00	32.12
ATOM	741	С	THR	1552	-11.282	11.419	13.591	1.00	32.74
ATOM	742	0	THR	1552	-11.171	12.525	13.057	1.00	35.26
ATOM	743	N	GLN	1553	-12.397	11.014	14.179	1.00	35.10
ATOM	745	CA	GLN	1553	-13.585	11.846	14.180	1.00 1.00	39.01
ATOM	746	CB	GLN	1553	-14.832	10.968	14.020	1.00	41.97
ATOM	747	CG	GLN	1553	-14.915	10.238	12.672	1.00	41.17
ATOM	748	CD	GLN	1553	-14.900	11.200	11.496	1.00	39.06
ATOM	749	OE1	GLN	1553	-15.785	12.045	11.359	1.00	41.84 41.92
ATOM	750	NE2	GLN	1553	-13.876	11.090	10.652	1.00	42.33
ATOM	<b>75</b> 3	C	GLN	1553	-13.727	12.777	15.372	1.00	45.35
ATOM	754	0	GLN	1553	-13.358	12.423	16.489	1.00	47.02
ATOM	755	N	ASP	1554	-14.225	13.981	15.090	1.00	48.60
ATOM	757	CA	ASP	1554	-14.479	15.016	16.084	1.00	50.64
ATOM	758	CB	ASP	1554	-15.832	14.766	16.758	1.00	54.52
ATOM	759	CG	ASP	1554	-17.003	14.955	15.809	1.00	60.54
ATOM ATOM	760	OD1	ASP	1554	-18.072	15.409	16.274	1.00	66.04
ATOM	761	OD2	ASP	1554	-16.860	14.661	14.601	1.00	65.09
ATOM	762 763	C	ASP	1554	-13.395	15.173	17.133	1.00	49.89
ATOM	764	0	ASP	1554	-13.611	14.879	18.310	1.00	51.48
ATOM	766	N	GLY	1555	-12.232	15.643	16.699	1.00	48.40
ATOM	767	CA	GLY	1555	-11.131	15.834	17.617	1.00	46.16
ATOM	768	C	GLY	1555	-9.798	15.626	16.935	1.00	44.64
ATOM	769	0	GLY	1555	-9.737	15.581	15.716	1.00	45.22
ATOM	770	N CD	PRO	1556	-8.708	15.525	17.702	1.00	44.68
	771	CA	PRO	1556	-8.672	15.683	19.164	1.00	45.39
	772	CB	PRO	1556	-7.359	15.326	17.177	1.00	42.95
	772 773	CG	PRO PRO	1556	-6.484	15.549	18.411	1.00	43.74
	. , ,		PRO	1556	-7.354	16.347	19.345	1.00	47 32

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MOTA	784	0	LEU	1557	-4.210	12.264	16.316	1.00	36.12
MOTA	785	N	TYR	1558	-5.664	10.539	16.292	1.00	32.49
ATOM	787	CA	TYR	1558	-4.861	9.697	17.157	1.00	31.87
MOTA	788	CB	TYR	1558	-5.590	9.348	18.470	1.00	33.93
MOTA	789	CG	TYR	1558	-5.695	10.476	19.471	1.00	35.34
ATOM	790	CD1	TYR	1558	-6.566	10.394	20.565	1.00	37.12
ATOM	791	CE1	TYR	1558	-6.683	11.456	21.479	1.00	36.44
ATOM	792	CD2	TYR	1558	-4.945	11.636	19.317	1.00	37.27
MOTA	793	CE2	TYR	1558	-5.054	12.690	20.213	1.00	39.62
MOTA	794	CZ	TYR	1558	-5.921	12.598	21.289	1.00	40.05
MOTA	795	OH	TYR	1558	-6.008	13.668	22.155	1.00	44.98
ATOM	797	C	TYR	1558	-4.600	8.419	16.387	1.00	31.58
ATOM	798	0	TYR	1558	-5.532	7.750	15.936	1.00	30.22
ATOM	799	N	VAL	1559	-3.331	8.129	16.153	1.00	33.43
ATOM	801	CA	VAL	1559	-2.947	6.907	15.463	1.00	31.42
ATOM	802	CB	VAL	1559	-1.849	7.160	14.419	1.00	32.31
ATOM	803	CG1	VAL	1559	-1.516	5.851	13.675	1.00	26.79
ATOM	804	CG2	VAL	1559	-2.308	8.265	13.453	1.00	30.63
MOTA	805	С	VAL	1559	-2.438	5.979	16.556	1.00	28.67
MOTA	806	0	VAL	1559	-1.393	6.223	17.155	1.00	30.08
ATOM	807	N	ILE	1560	-3.230	4.960	16.852	1.00	25.80
ATOM	809	CA	ILE	1560	-2.915	3.998	17.894	1.00	25.33
MOTA	810	CB	ILE	1560	-4.219	3.443	18.506	1.00	22.34
MOTA	811	CG2	ILE	1560	-3.931	2.695	19.784	1.00	20.36
ATOM	812	CG1	ILE	1560	-5.172	4.603	18.809	1.00	21.34
ATOM	813	CD1	ILE	1560	-6.583	4.190	19.093	1.00	20.68
ATOM	814	С	ILE	1560	-2.073	2.857	17.341	1.00	27.16
ATOM	815	0	ILE	1560	-2.520	2.116	16.455	1.00	29.67
ATOM	816	N	VAL	1561	0.858	2.714	17.860	1.00	27.69
ATOM	818	CA	VAL	1561	0.060	1.667	17.411	1.00	28.27
ATOM	819	CB	VAL	1561	1.311	2.269	16.696	1.00	27.34
ATOM	820	CG1	VAL	1561	0.892	3.019	15.445	1.00	21.76
ATOM	821	CG2	VAL	1561	2.074	3.201	17.639	1.00	26.00
ATOM	822	С	VAL	1561	0.509	0.809	18.588	1.00	28.70
ATOM	823	0	VAL	1561	0.221	1.139	19.746	1.00	30.52
ATOM	824	N	GLU	1562 1562	1.166	-0.311	18.286	1.00	28.64
ATOM ATOM	826 827	CA CB	GLU	1562	1.658	-1.220	19.318 18.693	1.00	27.77 24.57
ATOM	828	CG	GLU	1562	2.278 1.251	-2.465 -3.452	18.208	1.00	24.76
ATOM	829	CD	GLU	1562	1.864	-3.452 -4.641		1.00	27.27
ATOM	830	OE1	GLU	1562	1.272	-5.739	17.501 17.580	1.00	28.27
ATOM	831	OE1	GLU	1562	2.920	-4.487	16.849	1.00	29.25
ATOM	832	C	GLU	1562	2.674	-0.538	20.217	1.00	28.79
ATOM	833	0	GLU	1562	3.453	0.292	19.760	1.00	29.38
ATOM	834	N	TYR	1563	2.627	-0.871	21.503	1.00	30.84
ATOM	836	CA	TYR	1563	3.534	-0.304	22.493	1.00	31.43
ATOM	837	CB	TYR	1563	2.782	-0.088	23.799	1.00	32.10
ATOM	838	CG	TYR	1563	3.632	0.376	24.952	1.00	33.93
MOTA	839	CD1	TYR	1563	4.366	1.552	24.873	1.00	34.85
ATOM	840	CE1	TYR	1563	5.140	1.992	25.947	1.00	37.53
ATOM	841	CD2	TYR	1563	3.683	-0.356	26.136	1.00	34.81
ATOM	842	CE2	TYR	1563	4.452	0.072	27.211	1.00	34.01
ATOM	843	CZ	TYR	1563	5.173	1.245	27.113	1.00	35.79
ATOM	844	ОН	TYR	1563	5.920	1.677	28.184	1.00	39.10
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AT	'OM 84			LA 156					
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ATO			٠.	ER 1569	7.424				
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ATC						-1.949			
ATC						-3.271			
ATC		_	SE			-0.968			
ATO		-	SE			-0.219			35.56
ATO			LY			-1.673	26.243		38.69
ATO						-1.625	26.526		33.70
ATO						-3.033	26.530		31.40
ATO					11.555	-3.869	27.664		30.56
ATO					11.997	-5.308	27.599		32.32
ATO					11.632	-6.031	28.872	1.00	36.47 36.97
ATON		C	LYS		12.104	-7.436	28.804	1.00	41.62
ATON	1 874	ō	LYS	•	12.380	-0.664	25.683	1.00	32.18
ATOM	1 875	N	GLY		13.616	-0.691	25.715	1.00	32.57
ATOM		CA	GLY		11.686	0.223	24.973	1.00	33.39
ATOM	878	C	GLY		12.345	1.224	24.156	1.00	32.13
ATOM		ō	GLY		13.074	0.719	22.928	1.00	31.70
ATOM		N	ASN		12.912	-0.430	22.530	1.00	33.30
ATOM		CA	ASN		13.883	1.589	22.331	1.00	31.08
MOTA	883	CB	ASN	1568	14.632	1.230	21.139	1.00	31.00
ATOM	884	CG	ASN	1568	15.066	2.478	20.365	1.00	31.30
ATOM	885	OD1		1568	16.127	3.271	21.074	1.00	30.47
ATOM	886	ND2	ASN	1568	17.130 15.934	2.733	21.508	1.00	32.19
ATOM	889	С	ASN	1568	15.934	4.580	21.144	1.00	32.13
ATOM	890	0	ASN	1568	16.357	0.295	21.393	1.00	30.62
ATOM	891	N	LEU	1569	16.193	0.256	22.483	1.00	32.91
ATOM	893	CA	LEU	1569	17.269	-0.428	20.354	1.00	30.92
ATOM	894	CB	LEU	1569	17.418	-1.403	20.417	1.00	31.22
ATOM	895	CG	LEU	1569	18.415	-2.083 -3.231	19.054	1.00	29.57
ATOM	896	CD1	LEU	1569	18.284	-4.261	18.893		29.22
ATOM	897	CD2	LEU	1569	18.184	-3.863	20.024		21.30
ATOM	898	C	LEU	1569	18.609	-0.838	17.523		24.99
ATOM	899	0	LEU	1569	19.328		20.878		32.44
ATOM	900	N	ARG	1570	18.954		~ ~ ~ ~		33.12
ATOM ATOM	902	CA	ARG	1570	20.218				33.24
ATOM	903	CB	ARG	1570	20.348				33.01
ATOM	904	CG	ARG	1570	21.586				2.36
	905	CD	ARG	1570	21.672			_	8.28
ATOM	906	NE	ARG	1570	20.428				1.93
ATOM	908	CZ	ARG	1570	19.975				9.82
ATOM	909	NH1	ARG	1570	20.659				2.37
ATOM	912	NH2	ARG	1570	18.824				1.61
ATOM.	915	С	ARG	1570	20.308				3.28
ATOM ATOM	916	0	ARG	1570	21.184				3.90
ATOM	917	N	GLU	1571	19.359				3.17
						Z	22.981 1	00 3	3.45

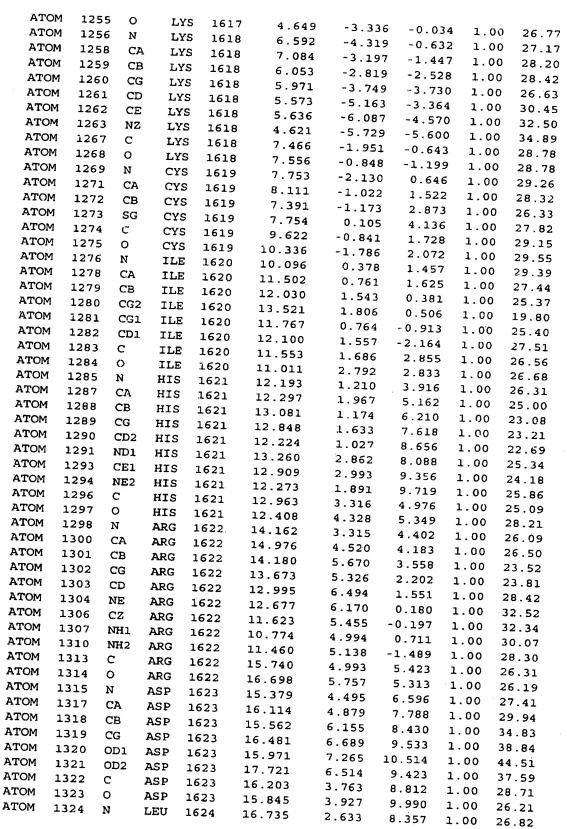
ATOM	919	CA	GLU	1571	19.284	1.861	24.432	1.00	34.87
MOTA	920	CB	GLU	1571	18.052	2.688	24.794	1.00	35.83
MOTA	921	CG	GLU	1571	18.158	4.145	24.354	1.00	41.61
MOTA	922	CD	GLU	1571	16.814	4.870	24.318	1.00	47.33
ATOM	923	OEl	GLU	1571	15.759	4.199	24.362	1.00	50.68
MOTA	924	OE2	GLU	1571	16.812	6.120	24.218	1.00	48.07
MOTA	925	С	GLU	1571	19.223	0.487	25.098	1.00	34.39
MOTA	926	0	GLU	1571	19.968	0.202	26.041	1.00	34.04
MOTA	927	N	TYR	1572	18.363	-0.376	24.572	1.00	33.49
MOTA	929	CA	TYR	1572	18.204	-1.728	25.083	1.00	30.45
MOTA	930	CB	TYR	1572	17.210	-2.495	24.202	1.00	28.13
MOTA	931	CG	TYR	1572	17.074	-3.971	24.487	1.00	25.80
MOTA	932	CD1	TYR	1572	16.105	-4.443	25.371	1.00	28.92
ATOM	933	CE1	TYR	1572	15.954	-5.804	25.618	1.00	30.03
ATOM	934	CD2	TYR	1572	17.899	-4.899	23.863	1.00	24.61
MOTA	935	CE2	TYR	1572	17.760	-6.260	24.102	1.00	26.05
ATOM	936	CZ	TYR	1572	16.790	-6.705	24.982	1.00	29.23
ATOM	937	OH	TYR	1572	16.651	-8.052	25.227	1.00	33.74
ATOM	939	С	TYR	1572	19.549	-2.447	25.113	1.00	31.30
MOTA	940	0	TYR	1572	19.880	-3.126	26.090	1.00	32.43
MOTA	941	N	LEU	1573	20.334	-2.266	24.058	1.00	29.68
MOTA	943	CA	LEU	1573	21.625	-2.923	23.972	1.00	30.04
ATOM	944	CB	LEU	1573	22.145	-2.909	22.529	1.00	26.13
ATOM	945	CG	LEU	1573	21.532	-3.870	21.490	1.00	25.24
ATOM	946	CD1	LEU	1573	22.097	-3.563	20.113	1.00	19.70
ATOM	947	CD2	LEU	1573	21.807	-5.317	21.839	1.00	22.05
ATOM	948	C	LEU	1573	22.645	-2.308	24.927	1.00	34.47
ATOM	949	0	LEU	1573	23.354	-3.031	25.644	1.00	34.95
ATOM	950	N C'D	GLN	1574	22.691	-0.980	24.978	1.00	35.47
ATOM ATOM	952 953	CA	GLN	1574	23.639	-0.293	25.850	1.00	37.09
ATOM	954	CB CG	GLN GLN	1574 1574	23.601 24.033	1.206 1.559	25.579 24.171	1.00	36.70 39.77
ATOM	955	CD	GLN	1574	23.960	3.045	23.884	1.00	41.51
ATOM	956	OE1	GLN	1574	23.592	3.837	24.751	1.00	42.57
ATOM	957	NE2	GLN	1574	24.288	3.431	22.652	1.00	41.34
ATOM	960	C	GLN	1574	23.400	-0.588	27.332	1.00	37.85
ATOM	961	0	GLN	1574	24.343	-0.801	28.090	1.00	38.87
ATOM	962	N ·	ALA	1575	22.131	-0.667	27.720	1.00	39.01
ATOM	964	CA	ALA	1575	21.740	-0.944	29.098	1.00	37.00
ATOM	965	СВ	ALA	1575	20.261	-0.678	29.273	1.00	35.71
ATOM	966	С	ALA	1575	22.061	-2.359	29.559	1.00	39.14
MOTA	967	0	ALA	1575	21.839	-2.692	30.719	1.00	43.81
ATOM	968	N	ARG	1576	22.563	-3.201	28.665	1.00	38.39
ATOM	970	CA	ARG	1576	22.897	-4.568	29.032	1.00	37.71
ATOM	971	CB	ARG	1576	21.994	-5.544	28.290	1.00	38.26
MOTA	972	CG	ARG	1576	20.555	-5.383	28.700	1.00	38.00
ATOM	973	CD	ARG	1576	19.653	-6.282	27.920	1.00	34.74
ATOM	974	NE	ARG	1576	18.279	-6.190	28.388	1.00	32.88
MOTA	976	CZ	ARG	1576	17.572	-5.066	28.442	1.00	34.02
MOTA	977	NH1	ARG	1576	18.114	-3.913	28.068	1.00	35.57
ATOM	980	NH2	ARG	1576	16.298	-5.102	28.800	1.00	36.71
ATOM	983	C	ARG	1576	24.365	-4.927	28.828	1.00	39.59
ATOM	984	0	ARG	1576	24.735	-6.113	28.788	1.00	39.83
ATOM	985	И	ARG	1577	25.200	-3.900	28.687	1.00	38.82

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AT				G 1577	26.63	1 -4.10	1 28.520	1 1 00	20
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ATO			ARC	1577					33.87
ATO			ARG	1577	27.72				33.06
ATO			ARG	1577	28.17				38.87
ATC				1577	28.68				39.76
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ATC			ARG	1577	27.18				43.26
ATO			ARG	1577	26.586				41.58
ATO			PRO		28.294				42.48
ATO			PRO	•	29.110			1.00	43.07
ATO			PRO	1578	28.839	-5.626			43.36
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ATO			PRO	1578	29.366		31.882	1.00	43.64
ATO		•	PRO	1578	29.530		31.215	1.00	43.37
ATO			PRO	1579	29.596		33.198	1.00 1.00	42.50
NOTA NOTA			PRO	1579	29.279		34.174	1.00	45.24
ATOM			PRO	1579	30.099	-3.187	33.882	1.00	44.69
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ATOM			PRO	1579	28.894	-4.615	35.361	1.00	45.78
ATOM			PRO	1579	31.548	-2.869	33.500	1.00	46.15
ATOM		_	PRO	1579	32.410	-3.753	33.478	1.00	48.38
ATOM			GLU	1592	19.022	-5.398	32.495	1.00	50.64 65.98
ATOM			GLU	1592	20.442	-5.048	32.492	1.00	64.80
ATOM			GLU	1592	20.796	-4.241	33.740	1.00	67.30
ATOM			GLU	1592	21.351	-6.275	32.371	1.00	63.80
ATOM	1021		GLU	1592	22.545	-6.149	32.089	1.00	65.21
ATOM		CA	GLU	1593	20.789	-7.458	32.607		61.44
ATOM		CB	GLU	1593	21.560	-8.691	32.495		60.82
ATOM		C	GLU	1593	20.681	-9.899	32.807		61.47
ATOM	1027	0	GLU	1593	22.144	-8.803	31.089		59.12
ATOM	1028	N	GLU GLN	1593	21.468	-8.525	30.097		59.49
ATOM	1030	CA	GLN	1594	23.408	-9.201	31.017	_	57.33
ATOM	1031	CB	GLN	1594 1594	24.103	-9.334	29 744		55.30
ATOM	1032	CG	GLN	1594	25.523	- 9.880	29.957		54.87
ATOM	1033	CD	GLN	1594	26.438	- <b>8.9</b> 59	30.757		53.34
ATOM	1034	OE1	GLN	1594	27.704	-9.660	31.248		55.27
ATOM	1035	NE2	GLN	1594	28.256	-10.536		1.00	6.47
ATOM	1038	C		1594	28.166	-9.275		1.00	1.46
MOTA	1039	0		1594	23.336	-10.229		1.00 5	2.29
ATOM	1040	N		1595	22.648	-11.166		1.00 5	2.56
ATOM	1042	CA		1595	23.447				9.40
ATOM	1043	CB		1595	22.783			1.00 4	6.00
MOTA	1044	CG		1595	22.452			1.00 4	2.94
ATOM	1045			1595	21.390			1.00 4	3.90
MOTA	1046		_	1595	21.495	_			9.46
ATOM	1047			1595	20.005			1.00 4	1.86
ATOM	1048			1595	23.741 24.950			1.00 4	3.96
ATOM	1049			1596	24.950				4.24
ATOM	1051			1596	24.076				3.29
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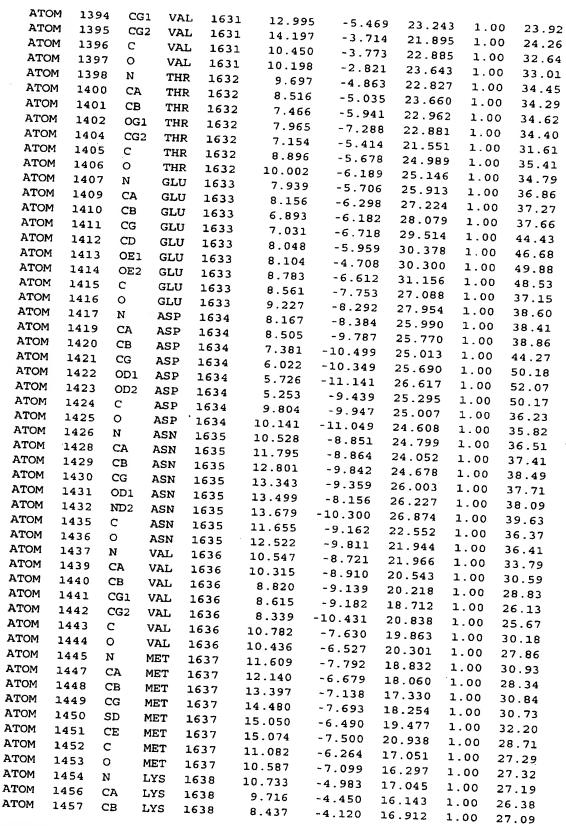
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MOTA	1056	0	SER	1596	23.857	-12.900	23.171	1.00	43.14	
MOTA	1057	N	SER	1597	25.277	-14.645	23.255	1.00	42.59	
MOTA	1059	CA	SER	1597	25.629	-14.553	21.850	1.00	42.91	
MOTA	1060	CB	SER	1597	26.739	-15.547	21.516	1.00	45.26	
MOTA	1061	OG	SER	1597	27.812	-15.436	22.431	1.00	56.41	
MOTA	1063	C	SER	1597	24.380	-14.909	21.048	1.00	42.35	
MOTA	1064	0	SER	1597	24.113	-14.322	20.003	1.00	43.71	
MOTA	1065	N	LYS	1598	23.621	-15.881	21.544	1.00	40.61	
MOTA	1067	CA	LYS	1598	22.405	-16.298	20.867	1.00	38.61	
MOTA	1068	CB	LYS	1598	21.848	-17.575	21.483	1.00	36.33	
ATOM	1069	CG	LYS	1598	21.135	-18.439	20.468	1.00	40.09	
ATOM	1070	CD	LYS	1598	20.213	-19.434	21.118	1.00	43.39	
ATOM	1071	CE	LYS	1598	19.766	-20.494	20.122	1.00	48.25	
MOTA	1072	NZ	LYS	1598	20.930	-21.290	19.623	1.00	50.46	
ATOM	1076	C:	LYS	1598	21.348	-15.194	20.895	1.00	38.17	
MOTA	1077	О	LYS	1598	20.579	-15.053	19.945	1.00	41.27	
MOTA	1078	N	ASP	1599	21.321	-14.408	21.969	1.00	35.90	
MOTA	1080	CA	ASP	1599	20.366	-13.307	22.099	1.00	34.08	
MOTA	1081	CB	ASP	1599	20.450	-12.661	23.477	1.00	37.83	
MOTA	1082	CG	ASP	1599	19.822	-13.505	24.562	1.00	39.93	
MOTA	1083	OD1	ASP	1599	20.089	-13.217	25.742	1.00	45.85	
MOTA	1084	OD2	ASP	1599	19.060	-14.444	24.240	1.00	41.06	
MOTA	1085	С	ASP	1599	20.634	-12.243	21.061	1.00	32.37	
ATOM	1086	0	ASP	1599	19.704	-11.701	20.466	1.00	32.58	
ATOM	1087	N	LEU	1600	21.915 <sup>.</sup>	-11.945	20.873	1.00	30.45	
ATOM	1089	CA	LEU	1600	22.355	-10.948	19.902	1.00	29.59	
ATOM	1090	CB	LEU	1600	23.841	-10.654	20.097	1.00	28.59	
ATOM	1091	CG	LEU	1600	24.238	-10.057	21.449	1.00	24.59	
ATOM	1092	CD1	<b>LEU</b>	1600	25.747	-9.869	21.522	1.00	18.40	
ATOM	1093	CD2	LEU	1600	23.529	-8.745	21.626	1.00	21.71	
ATOM	1094	C,	LEU	1600	22.073	-11.393	18.458	1.00	28.54	
ATOM	1095	O	LEU	1600	21.578	-10.613	17.648	1.00	25.59	
ATOM	1096	N	VAL	1601	22.377	-12.645	18.134	1.00	29.13	
ATOM	1098	CA	VAL	1601	22.111	-13.154	16.793	1.00	29.74	
MOTA	1099	CB	VAL	1601	22.780	-14.513	16.551	1.00	29.63	
MOTA	1100	CG1	VAL	1601	22.615	-14.922	15.105	1.00	29.30	
MOTA	1101	CG2	VAL	1601	24.259	-14.422	16.873	1.00	28.52	
ATOM	1102	С	VAL	1601	20.591	-13.247	16.564	1.00	29.98	
ATOM	1103	0	VAL	1601	20.106	-13.040	15.452	1.00	29.73	
ATOM	1104	N	SER	1602	19.855	-13.493	17.645	1.00	30.97	
ATOM	1106	CA	SER	1602	18.399	-13.576	17.607	1.00	29.64	
ATOM	1107	CB	SER	1602	17.894	-14.141	18.925	1.00	30.45	
MOTA	1108	OG	SER	1602	16.483	-14.158	18.962	1.00	39.63	
MOTA	1110	C	SER	1602	17.784	-12.192	17.343	1.00	29.30	
MOTA	1111	0	SER	1602	16.772	-12.071	16.641	1.00	28.74	
ATOM	1112	N	CYS	1603	18.385	-11.157	17.925	1.00	27.68	
MOTA	1114	CA	CYS	1603	17.931	-9.783	17.717	1.00	27.32	
MOTA	1115	CB	CYS	1603	18.791	-8.790	18.516	1.00	25.40	
ATOM	1116	SG	CYS	1603	18.472	-7.039	18.177	0.50	20.76	PRT1
MOTA	1117	С	CYS	1603	18.057	-9.468	16.225	1.00	28.34	
ATOM	1118	0	CYS	1603	17.134	-8.926	15.629	1.00	29.70	
MOTA	1119	N	ALA	1604	19.192	-9.837	15.627	1.00	29.36	

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ATO	OM 11:	21 C#	A AL	A 1604	19.43	9 0.50			
ATO		22 CE							
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ATO		25 N	TY						
ATO		7 CA			17.179				29.84
ATO	M 112	8 CB			17.107				28.26
ATO	M 112	9 CG		_	16.018				28.74
ATO	M 113				16.018	0,5			31.12
ATO					15.144	-0.230			32.53
ATO	M 113	2 CD:			14.853			1.00	30.84
ATO!	M 113	3 CE:			13.850			1.00	31.21
ATO	M 113	4 CZ	TYR		14.002		13.116	1.00	29.69
ATOM	1 113	5 OH	TYR		12.990		11.864	1.00	30.82
ATON	1 113	7 C	TYR		15.788		11.359	1.00	33.77
ATOM	1 1138	3 0	TYR		15.152		12.853	1.00	27.33
ATOM	1 .1139	N G	GLN		15.132	-11.691	11.805	1.00	27.94
ATOM	1 1141	CA	GLN	1606	14.008	-11.292	14.007	1.00	27.93
ATOM			GLN	1606	13.686	-10.659	_	1.00	27.20
ATOM	1143		GLN	1606	13.301	-10.335	15.570	1.00	26.40
ATOM			GLN	1606	13.301	-11.556	16.402	1.00	28.12
ATOM	1145	OE1		1606	12.188	-11.215	17.865	1.00	30.41
ATOM	1146	NE2		1606	14.008	-10.489	18.234	1.00	34.34
ATOM	1149	C	GLN	1606	13.906	-11.701	18.700	1.00	31.44
ATOM	1150	0	GLN	1606	12.884	-9.397	13.275	1.00	29.67
ATOM	1151	N	VAL	1607	14.970	-9.148	12.622	1.00	30.74
ATOM	1153	CA	VAL	1607	14.996	-8.602	13.281	1.00	29.59
MOTA	1154	CB	VAL	1607	16.235	-7.377	12.501	1.00	27.00
MOTA	1155	CG1	VAL	1607	16.382	-6.544 -5.307	12.842	1.00	27.20
ATOM	1156	CG2	VAL	1607	16.113	-5.397 -5.996	11.859	1.00	28.11
ATOM	1157	C	VAL	1607	14.966	-7.725	14.266	1.00	24.79
ATOM	1158	0	VAL	1607	14.229	-7.108	11.014	1.00	28:02
ATOM	1159	N	ALA	1608	15.736	-8.741	10.241	1.00	28.28
ATOM	1161	CA	ALA	1608	15.787	-9.206	10.626	1.00	27.56
ATOM	1162	CB	ALA	1608	16.801	-10.339	9.236		27.36
ATOM	1163	C	ALA	1608	14.402	-9.674	9.095		26.25
MOTA	1164	0	ALA	1608	14.013	-9.446	8.779 7.624		28.58
ATOM	1165	N	ARG	1609	13.660	-10.326	9.680		29.11
ATOM	1167	CA	ARG	1609	12.306	-10.797			28.88
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ATOM	1170	CD	ARG	1609	11.612				31.65
ATOM	1171	NE	ARG	1609	10.856				38.21
ATOM	1173	CZ	ARG	1609	10.048				11.10
ATOM	1174	NH1	ARG	1609	9.886				11.97
ATOM	1177	NH2	ARG	1609	9.411	-16.609			10.69
ATOM	1180	C	ARG	1609	11.312	-9.654		_	13.57
ATOM	1181	0		1609	10.480	-9.693			25.38
ATOM	1182	N	GLY	1610	11.365				15.75
ATOM	1184	CA	GLY	1610	10.480	-7.517			4.03
ATOM	1185	C	GLY	1610	10.734	-6.864			1.74
ATOM	1186	0	GLY	1610	9.805	-6.540	_		3.32
ATOM	1187	N	MET	1611	12.016	-6.714	_		3.39
ATOM	1189	CA	MET	1611	12.453	-6.125			4.48
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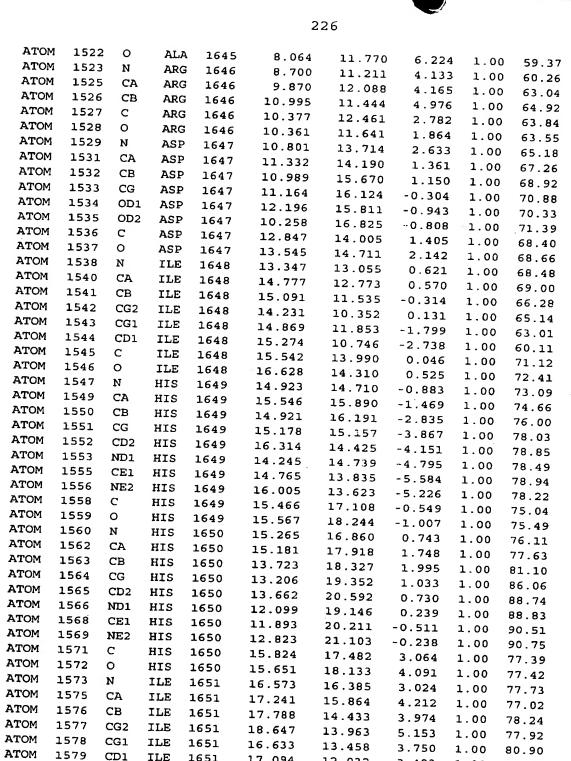
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MOTA	1192	SD	MET	1611	13.457	-3.123	7.536	1.00	25.27
MOTA	1193	CE	MET	1611	13.900	-2.801	5.876	1.00	22.25
ATOM	1194	С	MET	1611	12.100	-7.005	5.811	1.00	24.87
ATOM	1195	0	MET	1611	11.699	-6.497	4.755	1.00	24.09
ATOM	1196	N	GLU	1612	12.230	-8.321	5.975	1.00	25.48
MOTA	1198	CA	GLU	1612	11.894	-9.232	4.890	1.00	25.42
ATOM	1199	CB	GLU	1612	12.155	-10.691	5.288	1.00	23.41
MOTA	1200	CG	GLU	1612	11.664	-11.679	4.232	1.00	25.14
MOTA	1201	CD	GLU	1612	11.872	-13.141	4.599	1.00	28.60
ATOM	1202	OE1	GLU	1612	11.637	-13.514	5.777	1.00	30.10
ATOM	1203	OE2	GLU	1612	12.244	-13.928	3.694	1.00	29.53
ATOM	1204	C	GLU	1612	10.418	-9.021	4.521	1.00	26.92
ATOM	1205	0	GLU	1612	10.065	-8.928	3.343	1.00	29.61
ATOM	1206	N	TYR	1613	9.576	-8.884	5.542	1.00	27.88
MOTA	1208	CA	TYR	1613	8.154	-8.675	5.337	1.00	23.82
ATOM	1209	CB	TYR	1613	7.415	-8.769	6.667	1.00	24.17
ATOM	1210	CG	TYR	1613	5.941	-8.492	6.545	1.00	23.73
ATOM	1211	CD1	TYR	1613	5.064	-9.483	6.096	1.00	22.17
ATOM	1212	CE1	TYR	1613	3.698	-9.235	5.965	1.00	21.08
ATOM	1213	CD2	TYR	1613	5.419	-7.237	6.865	1.00	23.16
ATOM	1214	CE2	TYR	1613	4.054	-6.976	6.736	1.00	26.38
MOTA	1215	CZ	TYR	1613	3.200	-7.981	6.287	1.00	23.16
ATOM	1216	ОН	TYR	1613	1.855	-7.725	6.149	1.00	25.50
ATOM	1218	С	TYR	1613	7.885	-7.327	4.670	1.00	23.17
ATOM	1219	o	TYR	1613	7.147	-7.246	3.689	1.00	24.21
ATOM	1220	N	LEU	1614	8.481	-6.266	5.206	1.00	23.04
ATOM	1222	CA	LEU	1614	8.316	-4.920	4.652	1.00	21.81
ATOM	1223	CB	LEU	1614	9.107	-3.906	5.484	1.00	19.94
ATOM	1224	CG	LEU	1614	8.609	-3.616	6.902	1.00	21.94
ATOM	1225	CD1	LEU	1614	9.580	-2.719	7.654	1.00	14.28
ATOM	1226	CD2	LEU	1614	7.227	-2.977	6.814	1.00	17.45
MOTA	1227	C	LEU	1614	8.764	-4.858	3.182	1.00	23.74
ATOM	1228	0	LEU	1614	8.169	-4.150	2.367	1.00	25.26
ATOM	1229	N	ALA	1615	9.831	-5.587	2.862	1.00	25.00
ATOM	1231	CA	ALA	1615	10.357	-5.644	1.502	1.00	23.04
ATOM	1232	CB	ALA	1615	11.710	-6.360	1.483	1.00	20.02
ATOM	1233	C	ALA	1615	9.351	-6.357	0.605	1.00	23.15
ATOM	1234	0	ALA	1615	9.076	-5.891	-0.503	1.00	25.25
ATOM	1235	N	SER	1616	8.754	-7.441	1.104	1.00	23.64
ATOM	1237	CA	SER	1616	7.758	-8.199	0.337	1.00	23.60
ATOM	1238	CB	SER	1616	7.346	-9.453	1.107	1.00	22.46
ATOM	1239	OG	SER	1616	6.531	-9.131	2.224	1.00	26.66
ATOM	1241	С	SER	1616	6.505	-7.369	0.025	1.00	25.45
ATOM	1242	0	SER	1616	5.813	-7.607	-0.967	1.00	26.67
ATOM	1243	N	LYS	1617	6.193	-6.436	0.916	1.00	25.47
ATOM	1245	CA	LYS	1617	5.051	-5.551	0.781	1.00	25.04
ATOM	1246	СВ	LYS	1617	4.513	-5.183	2.163	1.00	26.30
ATOM	1247	CG	LYS	1617	3.778	-6.318	2.851	1.00	28.58
ATOM	1248	CD	LYS	1617	2.438	-6.530	2.169	1.00	33.00
MOTA	1249	CE	LYS	1617	1.652	-7.676	2.764	1.00	38.57
ATOM	1250	NZ	LYS	1617	2.167	-8.987	2.300	1.00	45.15
ATOM	1254	C	LYS	1617	5.417	-4.293	0.002	1.00	26.34
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ATOM	1326	CA	LEU	1624	16.905	1.469	9.216	1.00	25.91
ATOM	1327	CB	LEU:	1624	17.025	0.209	8.367	1.00	23.35
MOTA	1328	CG	LEU	1624	17.089	-1.107	9.127	1.00	21.09
MOTA	1329	CD1	LEU	1624	15.824	-1.303	10.009	1.00	14.44
MOTA	1330	CD2	LEU	1624	17.282	-2.215	8.101	1.00	18.30
ATOM	1331	C	LEU	1624	18.136	1.640	10.105	1.00	24.93
ATOM	1332	0	LEU	1624	19.235	1.897	9.611	1.00	25.58
MOTA	1333	N	ALA	1625	17.912	1.557	11.416	1.00	26.30
ATOM	1335	CA	ALA	1625	18.945	1.702	12.445	1.00	23.59
ATOM	1336	CB	ALA	1625	19.271	3.174	12.654	1.00	15.82
MOTA	1337	С	ALA	1625	18.351	1.116	13.732	1.00	23.64
ATOM	1338	0	ALA	1625	17.135	0.928	13.825	1.00	26.66
ATOM	1339	N	ALA	1626	19.197	0.815	14.712	1.00	21.59
MOTA	1341	CA	ALA	1626	18.708	0.266	15.974	1.00	21.66
ATOM	1342	CB	ALA	1626	19.860	-0.179	16.838	1.00	22.97
ATOM	1343	C	ALA	1626	17.835	1.272	16.731	1.00	24.98
MOTA	1.344	0	ALA	1626	17.072	0.891	17.620	1.00	26.84
ATOM	1345	N	ARG	1627	17.978	2.558	16.409	1.00	24.55
MOTA	1347	CA	ARG	1627	17.178	3.598	17.942	1.00	25.29
MOTA	1348	CB	ARG	1627	17.699	4.983	16.673	1.00	26.66
ATOM	1349	CG	ARG	1627	17.675	5.276	15.179	1.00	30.56
ATOM	1350	CD	ARG	1627	18.033	6.715	14.902	1.00	34.97
ATOM	1351	NE	ARG	1627	18.177	6.980	13.470	1.00	40.03
ATOM	1353	CZ	ARG	1627	19.322	6.864	12.809	1.00	40.62
ATOM	1354	NH1	ARG	1627	20.421	6.485	13.441	1.00	46.52
MOTA	1357	NH2	ARG	1627	19.377	7.159	11.523	1.00	43.25
ATOM	1360	C	ARG	1627	15.739				



ATOM	1458	CG	LYS	1638	7.702	-5.351	17.407	1.00	29.71
ATOM	1459	CD	LYS	1638	6.386	-5.018	18.109	1.00	31.48
MOTA	1460	CE	LYS	1638	5.485	-6.263	18.202	1.00	27.09
MOTA	1461	NZ	LYS	1638	4.888	-6.561	16.869	1.00	26.68
ATOM	1465	С	LYS	1638	10.196	-3.208	15.416	1.00	26.56
ATOM	1466	0	LYS	1638	10.514	-2.194	16.040	1.00	27.40
ATOM	1467	N	ILE	1639	10.211	-3.271	14.092	1.00	24.31
ATOM	1469	CA	ILE	1639	10.649	-2.147	13.289	1.00	24.84
ATOM	1470	CB	ILE	1639	10.924	-2.588	11.836	1.00	25.81
ATOM	1471	CG2	ILE	1639	11.248	-1.395	10.952	1.00	24.18
ATOM	1472	CG1	ILE	1639	12.094	-3.566	11.826	1.00	25.01
MOTA	1473	CD1	ILE	1639	12.075	-4.499	10.675	1.00	27.90
MOTA	1474	C	ILE	1639	9.641	-0.999	13.348	1.00	24.90
MOTA	1475	0	ILE	1639	8.435	-1.186	13.170	1.00	25.24
ATOM	1476	N	ALA	1640	10.167	0.183	13.635	1.00	25.70
ATOM	1478	CA	ALA	1640	9.378	1.392	13.744	1.00	27.61
ATOM	1479	CB	ALA	1640	9.699	2.094	15.070	1.00	26.37
ATOM	1480	C	ALA	1640	9.637	2.348	12.576	1.00	28.35
ATOM	1481	0	ALA	1640	10.650	2.243	11.871	1.00	28.40
ATOM	1482	N	ASP	1641	8.676	3.237	12.354	1.00	29.74
ATOM	1484	CA	ASP	1641	8.760	4.272	11.325	1.00	32.13
ATOM	1485	CB	ASP	1641	9.873	5.273	11.688	1.00	34.31
ATOM	1486	CG	ASP	1641	9.507	6.158	12.896	1.00	36.31
ATOM	1487	OD1	ASP	1641	10.299	7.056	13.258	1.00	42.18
MOTA	1488	OD2	ASP	1641	8.420	5.974	13.483	1.00	41.03
MOTA	1489	C	ASP	1641	8.882	3.840	9.867	1.00	32.00
ATOM	1490	0	ASP	1641	9.339	4.617	9.021	1.00	32.65
MOTA	1491	N	PHE	1642	8.415	2.634	9.563	1.00	30.61
ATOM	1493	CA	PHE	1642	8.473	2.119	8.200	1.00	30.06
ATOM'	1494	CB	PHE	1642	8.248	0.606	8.189	1.00	24.46
ATOM	1495	CG	PHE	1642	6.981	0.176	8.854	1.00	23.26
ATOM	1496	CD1	PHE	1642	5.799	0.075	8.125	1.00	19.66
ATOM	1497	CD2	PHE	1642	6.9 <b>6</b> 6	-0.134	10.209	1.00	22.88
ATOM	1498	CEl	PHE	1642	4.609	-0.331	8.734	1.00	20.97
ATOM	1499	CE2	PHE	1642	5.785	-0.540	10.830	1.00	26.61
ATOM	1500	CZ	PHE	1642	4.599	-0.639	10.083	1.00	24.82
ATOM	1501	С	PHE	1642	7.512	2.830	7.225	1.00	33.14
MOTA	1502	0	PHE	1642	7.791	2.922	6.029	1.00	36.48
ATOM	1503	N	GLY	1643	6.411	3.372	7.741	1.00	32.65
ATOM	1505	CA	GLY	1643	5.462	4.059	6.876	1.00	32.28
ATOM	1506	С	GLY	1643	5.629	5.560	6.913	1.00	32.19
ATOM	1507	0	GLY	1643	4.795	6.310	6.415	1.00	30.74
ATOM	1508	N	LEU	1644	6.739	5.997	7.486	1.00	36.80
ATOM	1510	CA	LEU	1644	7.052	7.406	7.630	1.00	41.95
ATOM	1511	CB	LEU	1644	8.332	7.551	8.439	1.00	37.41
ATOM	1512	CG	LEU	1644	8.377	8.746	9.369	1.00	38.98
ATOM	1513	CD1	LEU	1644	7.384	8.548	10.493	1.00	40.45
ATOM	1514	CD2	LEU	1644	9.775	8.904	9.929	1.00	41.94
ATOM	1515	С	LEU	1644	7.189	8.150	6.296	1.00	47.55
MOTA	1516	0	LEU	1644	7.787	7.648	5.341	1.00	50.55
ATOM	1517	N	ALA	1645	6.637	9.356	6.247	1.00	52.59
ATOM	1519	CA	ALA	1645	6.686	10.194	5.055	1.00	56.88
ATOM	1520	CB	ALA	1645	5.391	10.999	4.942	1.00	58.01
ATOM	1521	С	ALA	1645	7.880	11.135	5.178	1.00	58.95



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20.216

12.032

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17.078

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18.781

19.499

3.483

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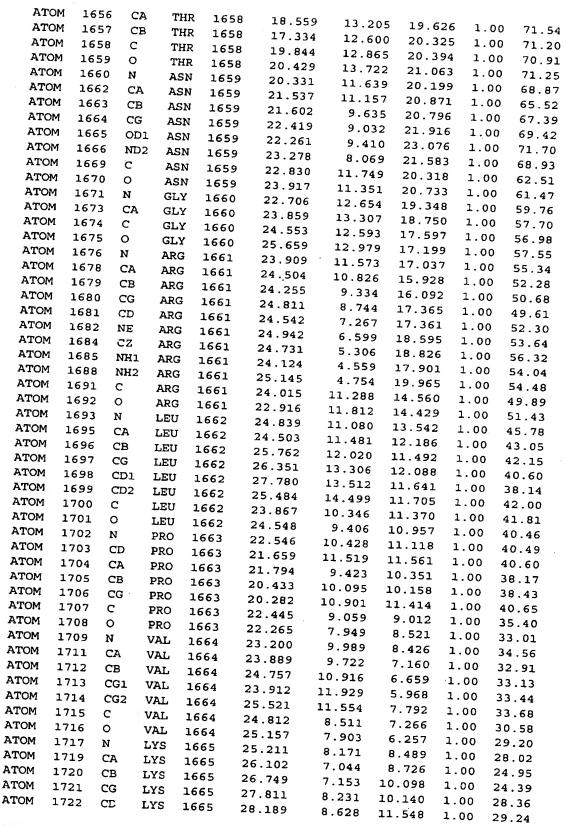
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1.00 MOTA 1587 OD1 ASP 1652 19.786 7.636 82.38 21.247 MOTA 1588 OD2 ASP 1.00 1652 20.081 19.780 9.497 81.51 MOTA 1589 С ASP 1652 20.637 16.984 6.783 1.00 72.31 **ATOM** 1590 0 ASP 1652 20.599 16.403 7.866 1.00 71.41 **ATOM** 1591 N TYR 1653 21.610 16.805 5.894 1.00 71.44 **ATOM** 1593 CA TYR 1653 22.736 15.900 6.143 1.00 70.07 MOTA 1594 CB TYR 1653 23.655 15.849 4.921 1.00 66.96 **ATOM** 1595 TYR CG 1653 23.153 14.932 3.834 1.00 66.43 ATOM 1596 CD1 TYR 1653 23.881 14.757 2.657 1.00 66.60 **ATOM** 1597 CE1 TYR 1653 23.434 13.898 1.653 1.00 68.33 ATOM 1598 CD2 TYR 1653 21.960 14.224 3.981 1.00 66.58 ATOM 1599 CE2 TYR 1653 21.500 13.363 2.990 1.00 68.84 **ATOM** 1600 CZTYR 1653 22.241 13.205 1.823 1.00 69.34 ATOM 1601 OH TYR 1653 21.781 12.360 0.833 1.00 69.88 ATOM 1603 C TYR 1653 23.557 16.227 7.391 1.00 70.80 MOTA 1604 0 TYR 1653 24.197 15.351 7.975 1.00 70.62 **ATOM** 1605 N TYR 1654 23.531 17.488 7.802 1.00 70.76 MOTA 1607 CA TYR 1654 24.280 17.902 8.972 1.00 70.97 ATOM 1608 CB TYR 1654 24.795 19.328 8.783 1.00 69.27 MOTA 1609 CĠ TYR 1654 25.935 19.401 7.787 1.00 69.68 MOTA 1610 CD1 TYR 1654 25.696 19.352 6.415 1.00 69.51 MOTA 1611 CE1 TYR 1654 26.750 19.380 5.498 1.00 70.15 **ATOM** 1612 CD2 TYR 1654 27.256 19.482 8.221 1.00 69.92 **ATOM** 1613 CE2 TYR 1654 28.314 19.513 7.316 1.00 70.26 ATOM 1614 CZTYR 1654 28.057 19.462 5.958 1.00 70.22 **ATOM** 1615 OH TYR 1654 29.111 19.492 5.069 1.00 69.67 ATOM 1617 TYR 17.763 С 1654 23.503 10.272 1.00 72.19 MOTA 1618 O TYR 24.035 1654 18.043 11.344 1.00 73.21 **ATOM** 1619 N LYS 1655 22.269 17.275 10.183 1.00 73.05 **ATOM** 1621 74.81 CA LYS 1655 21.424 17.108 11.363 1.00 **ATOM** 1622 CB LYS 19.955 1655 17.124 10.953 1.00 75.63 **ATOM** 1623 CG LYS 18.978 1655 17.239 12.102 1.00 79.16 **ATOM** 1624 CD LYS 1655 17.581 17.513 11.576 1.00 84.09 **ATOM** 1625 CE LYS 1655 16.517 17.244 12.634 1.00 87.56 MOTA 1626 NZ LYS 1655 15.139 17.478 12.097 1.00 89.36 **ATOM** 1630 C LYS 1655 21.738 15.834 12.156 1.00 75.72 **ATOM** 1631 0 LYS 1655 21.900 14.751 11.586 1.00 77.14 **ATOM** 1632 N LYS 1656 21.815 15.977 1.00 75.08 13.477 **ATOM** 1634 CA LYS 1656 22.106 14.857 14.363 1.00 73.36 MOTA 1635 CB LYS 1656 23.062 15.296 15.477 1.00 72.88 ATOM 1636 CG LYS 1656 24.475 15.599 15.007 1.00 72.87 MOTA 1637 LYS CD 1656 25.346 16.048 16.167 1.00 74.66 **ATOM** 1638 CE LYS 1656 26.830 15.945 15.828 1.00 74.84 **ATOM** 1639 NZ LYS 1656 27.701 16.322 16.981 1.00 73.74 **ATOM** 1643 С LYS 1656 20.827 14.311 14.982 1.00 72.45 ATOM 1644 0 LYS 1656 19.795 14.991 15.007 1.00 72.74 MOTA 1645 N THR 1657 20.900 13.075 15.469 1.00 71.26 MOTA 1647 CA THR 1657 19.763 12.426 16.107 1.00 70.05 ATOM 1648 CB THR 1657 19.969 10.886 16.206 1.00 68.30 ATOM 1649 OG1 THR 1657 21.084 10.598 17.060 1.00 69.34 MOTA 1651 CG<sub>2</sub> THR 1657 20.244 10.292 14.B39 1.00 66.16 **ATOM** 1652 С THR 1657 19.707 13.019 17.504 1.00 70.37 **ATOM** 1653 0 THR 1657 20.608 13.761 17.892 1.00 71.47 MOTA 1654 N THR 1658 18.669 12.691 18.263 1.00 70.80



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MOTA 9.690 11.489 1.00 1723 CE LYS 1665 29.269 31.15 29.639 MOTA NZ 10.194 12.836 1.00 1724 LYS 1665 35.47 MOTA 1728 C LYS 1665 25.440 5.692 8.543 1.00 25.16 MOTA 1729 0 LYS 1665 26.096 4.671 8.627 1.00 24.34 MOTA 1730 N TRP 1666 24.138 5.698 8.286 1.00 25.16 MOTA 1732 CA TRP 1666 23.414 4.461 8.053 1.00 26.61 ATOM 1733 TRP CB 1666 22.157 4.412 8.917 1.00 28.17 ATOM TRP 1734 CG 1666 22.428 3.931 10.330 1.00 30.26 MOTA 1735 CD2 TRP 1666 22.930 4.714 11.426 1.00 26.92 **ATOM** 1736 TRP CE2 1666 23.063 3.837 12.537 1.00 26.34 MOTA 1737 CE3 TRP 1666 6.057 23.286 11.598 1.00 24.69 MOTA 1738 CD1 TRP 1666 22.276 2.656 10.800 1.00 26.44 MOTA 1739 TRP NE1 1666 22.659 2.592 12.118 1.00 25.65 **ATOM** 1741 CZ2 TRP 1666 23.535 4.264 13.779 1.00 24.97 **ATOM** 1742 CZ3 TRP 1666 23.758 6.484 12.837 1.00 22.23 **ATOM** 1743 CH2 TRP 1666 23.877 5.587 13.908 1.00 24.97 MOTA 1744 C TRP 1666 23.048 4.345 6.572 1.00 27.24 1745 **ATOM** TRP 0 1666 22.573 3.301 6.116 1.00 29.16 ATOM 1746 N MET 1667 23.355 5.390 5.811 1.00 26.70 ATOM 1748 CA MET 1667 23.022 5.444 4.398 1.00 25.21 MOTA 1749 CB MET 1667 22.828 6.893 3.963 1.00 28.81 1750 MOTA CG MET 1667 21.704 7.630 4.637 1.00 35.42 MOTA 1751 SD MET 1667 21.567 9.283 3.924 1.00 42.64 ATOM 1752 CE MET 1667 20.959 8.858 2.369 1.00 41.32 ATOM 1753 С MET 1667 23.984 4.807 3.417 1.00 25.03 MOTA 1754 0 MET 1667 25.182 5.047 3.446 1.00 24.24 MOTA 1755 N ALA 1668 23.420 4.034 2.501 1.00 26.70 MOTA 1757 CA ALA 1668 24.186 3.398 1.441 1.00 27.82 MOTA 1758 CB ALA 1668 23.272 2.509 0.601 1.00 25.36 MOTA 1759 С ALA 1668 24.738 4.528 0.575 1.00 28.42 ATOM 1760 0 ALA 1668 24.044 5.521 0.321 1.00 27.52 MOTA 1761 N PRO 1669 25.972 4.374 0.065 1.00 28.95 ATOM 1762 CD PRO 1669 26.867 3.214 0.170 1.00 27.98 MOTA 1763 CA PRO 1669 26.571 5.418 -0.775 1.00 28.76 MOTA 1764 CB PRO 1669 27.814 4.731 -1.326 1.00 28.58 MOTA 1765 CG PRO 1669 28.193 3.809 -0.209 1.00 30.22 MOTA 1766 C PRO 1669 25.647 5.909 -1.8931.00 27.08 **ATOM** 1767 0 PRO 1669 25.496 7.107 -2.093 1.00 28.31 ATOM 1768 N GLU 1670 24.993 4.997 -2.595 1.00 25.42 ATOM 1770 CA GLU 1670 24.110 5.423 -3.673 1.00 27.02 MOTA 1771 CB GLU 1670 23.680 4.233 -4.542 1.00 27.18 **ATOM** 1772 CG GLU 1670 22.662 3.294 -3.911 1.00 27.66 **ATOM** 1773 CD GLU 1670 23.280 2.162 -3.112 1.00 27.75 MOTA OE1 1774 GLU 1670 22.488 1.309 -2.647 1.00 27.12 MOTA 1775 OE2 GLU 1670 24.526 2.114 -2.944 1.00 21.64 **ATOM** 1776 C GLU 1670 22.896 6.229 -3.189 1.00 26.88 ATOM 1777 0 GLU 1670 22.348 7.037 -3.929 1.00 24.52 MOTA -1.948 1.00 1778 N ALA 1671 22.477 6.009 29.43 MOTA 1780 CA ALA 1671 21.342 6.744 -1.392 1.00 29.29 **ATOM** 1781 CB ALA 1671 20.751 5.989 -0.217 1.00 26.98 MOTA 1782 C ALA 1671 21.826 8.124 -0.939 1.00 31.14 ATOM 1783 0 ALA 1671 21.159 9.135 -1.143 1.00 31.67 MOTA 1784 N LEU 1672 23.013 8.139 -0.343 1.00 32.31 MOTA 1786 LEU 1672 CA 23.636 9.352 0.154 1.00 33.79



ATO	M 170	7 00							
ATO				_	24.841	8.986	1.008	3 1.00	34.49
ATO					25.585	10.166	1.618		
ATO					24.713	10.840			
				_	26.863	9.665			
ATO.		_	LEU	J 1672	24.078	10.280			
ATO		_	LEU	J 1672	23.789	11.478			
ATO			PHE	1673	24.770	9.723			
ATO			PHE	1673	25.266	10.504			
ATO			PHE	1673	26.553	9.874			33.81
ATO			PHE	1673	27.661	9.761	_		33.15
ATON			PHE	1673	28.313	8.545			33.44
ATON			PHE	1673	28.055	10.867			32.17
ATOM			PHE	1673	29.346	8.419	-1.484		34.87
ATOM		CE2	PHE		29.090	10.757		1.00	31.98
ATOM			PHE	1673	29.736	9.525	-0.919	1.00	36.31
ATOM		C	PHE	1673	24.273	10.670	-0.732	1.00	34.55
ATOM		0	PHE	1673	24.135	11.754	-4.217	1.00	34.79
ATOM		N	ASP	1674	23.584	9.588	-4.765	1.00	35.74
ATOM		CA	ASP	1674	22.650	9.601	-4.572	1.00	37.31
ATOM	1808	CB	ASP	1674	22.917		-5.698	1.00	35.61
ATOM	1809	CG	ASP	1674	24.362	8.392	-6.600	1.00	37.01
ATOM	1810	OD1	ASP	1674	25.030	8.288	-7.041	1.00	41.02
MOTA	1811	OD2	ASP	1674	24.828	9.340	-7.194	1.00	43.07
MOTA	1812	C	ASP	1674	21.162	7.145	-7.251	1.00	42.24
MOTA	1813	0	ASP	1674	20.315	9.632	-5.360	1.00	37.06
ATOM	1814	N	ARG	1675	20.840	9.506	-6.257	1.00	36.37
MOTA	1816	CA	ARG	1675	19.445	9.745	-4.077	1.00	37.78
ATOM	1817	CB	ARG	1675	18.832	9.791	-3.650	1.00	39.41
ATOM	1818	CG	ARG	1675		11.137	-4.039	1.00	44.39
ATOM	1819	CD	ARG	1675	19.413	12.299	-3.269	1.00	54.30
ATOM	1820	NE	ARG	1675	19.516	13.551	-4.127	1.00	63.84
ATOM	1822	CZ	ARG	1675	20.060	14.664	-3.349	1.00	73.69
ATOM	1823	NH1	ARG	1675	19.652	15.925	-3.453	1.00	77.10
ATOM	1826	NH2	ARG	1675	18.695	16.253	-4.312	1.00	79.65
ATOM	1829	C	ARG	1675	20.177	16.855	-2.665	1.00	79.31
ATOM	1830	Ö	ARG		18.617	8.639	-4.221	1.00	37.46
ATOM	1831	N	ILE	1675	17.447	8.808	4.557	1.00	38.57
ATOM	1833	CA	ILE	1676	19.235	7.475	-4.351	1.00	34.37
ATOM	1834	CB	ILE	1676	18.545	6.313	-4.874	1.00	32.99
ATOM	1835	CG2		1676	19.358	5.644	-5.976	1.00	33.98
ATOM	1836	CG1	ILE	1676	18.552	4.529	-6.602	1.00	35.04
ATOM	1837	CD1	ILE	1676	19.708	6.663	-7.050	1.00	34.92
ATOM	1838	CDI	ILE	1676	20.799	6.200	-7.962	1.00	41.16
ATOM	1839	0	ILE	1676	18.315	5.315	-3.743		31.55
ATOM	1840		ILE	1676	19.245	4.632	-3.300		30.65
ATOM	1842	N	TYR	1677	17.082	5.279	-3.246		30.88
ATOM		CA	TYR	1677	16.701	4.371	-2.173		27.10
ATOM	1843	CB	TYR	1677	15.771	5.074			28.30
	1844	CG	TYR	1677	16.457	6.136			30.61
ATOM	1845	CD1	TYR	1677	16.598	7.432	-0.905		30.82
ATOM	1846	CE1	TYR	1677	17.212	8.424			30.82
ATOM	1847	CD2		1677	16.952	5.857			
ATOM	1848	CE2		1677	17.567	6.842			29.75
ATOM	1849	CZ		1677	17.688	8.125			32.62
MOTA	1850	ОН	TYR	1677	18.238	9.118			34.51
							2.000	1.00 .	38.89



ATOM	1852	С	TYR	1677	16.029	3.149	-2.743	1.00	25.47
ATOM	1853	0	TYR	1677	15.132	3.264	-3.578	1.00	26.00
MOTA	1854	N	THR	1678	16.459	1.983	-2.272	1.00	24.27
ATOM	1856	CA	THR	1678	15.942	0.701	-2.734	1.00	24.09
MOTA	1857	CB	THR	1678	16.830	0.123	-3.853	1.00	24.19
ATOM	1858	OG1	THR	1678	18.165	-0.008	-3.349	1.00	27.81
ATOM	1860	CG2	THR	1678	16.843	1.009	-5.085	1.00	24.15
ATOM	1861	C	THR	1678	15.979	-0.297	-1.577	1.00	25.02
ATOM	1862	0	THR	1678	16.379	0.036	-0.465	1.00	27.65
ATOM	1863	N	HIS	1679	15.569	-1.530	-1.844	1.00	25.04
ATOM	1865	CA	HIS	1679	15.591	-2.560	-0.818	1.00	24.35
MOTA	1866	CB	HIS	1679	14.853	-3.812	-1.298	1.00	23.78
MOTA	1867	CG	HIS	1679	13.390	-3.592	-1.536	1.00	27.24
MOTA	1868	CD2	HIS	1679	12.627	-3.758	-2.643	1.00	28.22
MOTA	1869	ND1	HIS	1679	12.532	-3.137	-0.551	1.00	30.64
ATOM	1871	CE1	HIS	1679	11.310	-3.028	-1.041	1.00	28.13
ATOM	1872	NE2	HIS	1679	11.339	-3.400	-2.307	1.00	28.52
ATOM	1874	C	HIS	1679	17.056	-2.846	-0.514	1.00	22.52
ATOM	1875	0	HIS	1679	17.419	-3.179	0.613	1.00	22.58
ATOM	1876	N	GLN	1680	17.898	-2.604	-1.516	1.00	24.34
ATOM	1878	CA	GLN	1680	19.341	-2.800	-1.406	1.00	23.52
ATOM	1879	CB	GLN	1680	19.998	-2.781	-2.782	1.00	25.36
ATOM	1880	CG	GLN	1680	19.741	-4.050	-3 577	1.00	33.28
ATOM	1881	CD	GLN	1680	19.212	-3.763	-4.949	1.00	34.68
ATOM	1882	OE1	GLN	1680	18.683	-2.686	-5.187	1.00	41.24
ATOM	1883	NE2	GLN	1680	19.357	-4.713	-5.867	1.00	32.10
MOTA	1886	C	GLN	1680	19.998	-1.767	-0.514	1.00	23.38
ATOM	1887	0	GLN	1680	20.925	-2.094	0.224	1.00	25.12
ATOM	1888	N	SER	1681	19.533	-0.521	-0.562	1.00	20.87
ATOM	1890	CA	SER	1681	20.133	0.480	0.303	1.00	20.53
ATOM	1891	CB	SER	1681	19.821	1.919	-0.151	1.00	19.58
ATOM ATOM	1892	OG C	SER	1681	18.445	2.126	-0.425	1.00	20.67
ATOM	1894 1895	0	SER	1681	19.696	0.189	1.741	1.00	22.22
ATOM	1896		SER	1681	20.439	0.455	2.681	1.00	23.62
ATOM	1898	N CA	ASP	1682	18.530	-0.436	1.900	1.00	22.44
ATOM	1899	CB	ASP ASP	1682 1682	18.054	-0.816	3.231	1.00	22.70
ATOM	1900	CG	ASP	1682	16.607	-1.293	3.180	1.00	24.24
ATOM	1901	OD1	ASP	1682	15.603 14.410	-0.165	3.352	1.00	28.23
ATOM	1902	OD2	ASP	1682	15.976	-0.425 0.960	3.108 3.757	1.00	28.14
ATOM	1903	C	ASP	1682	18.926	-1.941	3.777	1.00	25.23
ATOM	1904	ō	ASP	1682	19.121	-2.057	4.990	1.00	23.92
ATOM	1905	N	VAL	1683	19.433	-2.788	2.884	1.00	26.24
ATOM	1907	CA	VAL	1683	20.300	-3.888	3.302	1.00	23.67
ATOM	1908	СВ	VAL	1683	20.562	-4.881	2.141	1.00	22.42
ATOM	1909	CG1	VAL	1683	21.724	-5.802	2.459	1.00	23.70
ATOM	1910	CG2	VAL	1683	19.292	-5.713	1.889	1.00	19.73 19.85
ATOM	1911	C	VAL	1683	21.584	-3.298	3.860	1.00	
ATOM	1912	0	VAL	1683	22.030	-3.688	4.938	1.00	21.94
ATOM	1913	N	TRP	1684	22.141	-2.320	3.154	1.00	22.69 20.51
ATOM	1915	CA	TRP	1684	23.349	-1.633	3.611	1.00	20.31
ATOM	1916	CB	TRP	1684	23.659	-0.446	2.680	1.00	19.01
MOTA	1917	CG	TRP	1684	24.802	0.410	3.145	1.00	20.67
ATOM	1918	CD2	TRP	1684	26.114	0.468	2.587	1.00	22.26
						0.400	2.JU,		

ATC	M 191	9 CE:	2 11121						
ATO			_	·			5 3.408	3 1.00	21.22
ATO					26.718			3 1.00	
ATO					24.825	1.229	4.248		
ATO					26.079	1.763	4.414		
ATO					28.236	1.586			
ATO				· · · ·	28.059	0.141			
					28.806	0.992			
ATO		_	TRP	1684	23.131	-1.150			
ATO		_	TRP	1684	23.958	-1.412		•	
ATO		N	SER	1685	22.015	-0.463			
OTA		. CA	SER	1685	21.652	0.042			
MOTA		CB	SER		20.310	0.773		1.00	20.02
ATON	1 1933	OG	SER	1685	20.335	1.791			19.12
NOTA		C	SER	1685	21.551	-1.111		1.00	21.62
ATOM	1 1936	0	SER	1685	21.908	-0.946	7.648	1.00	22.64
MOTA	1 1937	N	PHE	1686	21.043		8.829	1.00	22.09
ATOM	1 1939	CA	PHE	1686	20.939	-2.266	7.202	1.00	22.44
ATOM	1940	CB	PHE	1686	20.196	-3.438	8.075	1.00	22.91
ATOM		CG	PHE	1686		-4.588	7.380	1.00	23.75
ATOM	1942	CD1	PHE	1686	20.027	-5.808	8.256	1.00	23.61
ATOM		CD2	PHE	1686	19.220	-5.757	9.388	1.00	21.21
ATOM		CE1	PHE		20.731	-6.976	7.990	1.00	23.91
ATOM		CE2	PHE	1686	19.118	-6.836	10.240	1.00	20.66
ATOM		CZ	PHE	1686	20.636	-8.074	8.841	1.00	22.47
ATOM	•	C	PHE	1686	19.828	-7.999	9.972	1.00	23.35
ATOM		o o		1686	22.339	-3.904	8.522	1.00	22.60
ATOM	1949	N	PHE	1686	22.526	-4.382	9.646	1.00	22.83
ATOM	1951		GLY	1687	23.312	-3.770	7.626	1.00	23.82
ATOM	1952	CA	GLY	1687	24.682	-4.140	7.941	1.00	22.58
ATOM	1953	C	GLY	1687	25.175	-3.262	9.071	1.00	21.49
ATOM		0	GLY	1687	25.832	-3.749	9.990	1.00	21.62
ATOM	1954	N	VAL	1688	24.849	-1.968	9.008	1.00	21.15
ATOM	1956	CA	VAL	1688	25.229	-1.008	10.052	1.00	20.56
ATOM	1957	CB	VAL	1688	24.894	0.479	9.647	1.00	17.69
ATOM	1958	CG1	VAL	1688	25.408	1.456	10.690	1.00	15.11
ATOM	1959	CG2	VAL	1688	25.518	0.821	8.314	1.00	11.54
	1960	C	VAL	1688	24.494	-1.398	11.346	1.00	22.60
ATOM	1961	0	VAL	1688	25.083	-1.407	12.428	1.00	25.23
ATOM	1962	N	LEU	1689	23.215	-1.755	11.229	1.00	26.09
ATOM	1964	CA	LEU	1689	22.423	-2.175	12.387	1.00	
ATOM	1965	CB	LEU	1689	20.976	-2.455	11.965	1.00	25.16 25.91
ATOM	1966	CG	LEU	1689	19.913	-2.560	13.068	1.00	
ATOM	1967	CD1	LEU	1689	18.557	-2.241	12.496	1.00	27.54
ATOM	1968	CD2	LEU	1689	19.898	-3.940	13.704	1.00	28.11
MOTA	1969	С	LEU	1689	23.055	-3.426	13.704		31.67
ATOM	1970	0	LEU	1689	23.128	-3.532			27.49
ATOM	1971	N	LEU	1690	23.485	-4.374	14.246	1.00	28.99
ATOM	1973	CA	LEU	1690	24.149		12.180		27.67
ATOM	1974	CB	LEU	1690	24.616	-5.596	12.643		26.76
ATOM	1975		LEU	1690	23.651	·6.453	11.456		28.58
ATOM	1976		LEU	1690		-7.406	10.733		29.46
ATOM	1977			1690	24.372	-8.064			27.79
ATOM	1978				23.130	-8.488		1.00	28.15
ATOM	1979			1690	25.362	-5.176		1.00	26.19
ATOM	1980			1690	25.565		14.597		25.29
	2200	7.4	IKP	1691	26.124	-4.217	12.946		25.89
CCC - 1									

7	MOTA	1982	CA	TRP	1691	27.302	-3.682	13.631	1.00	27.31
1	MOTA	1983	CB	TRP	1691	27. <b>97</b> 9	-2.628	12.755	1.00	25.21
1	MOTA	1984	CG	TRP	1691	29.338	-2.170	13.257	1.00	27.00
7	MOTA	1985	CD2	TRP	1691	29.606	-1.060	14.134	1.00	24.28
7	MOTA	1986	CE2	TRP	1691	31.001	-0.988	14.297	1.00	23.03
1	MOTA	1987	CE3	TRP	1691	28.792	-0.118	14.778	1.00	22.80
7	MOTA	1988	CD1	TRP	1691	30.562	-2.712	12.944	1.00	24.10
7	MOTA	1989	NE1	TRP	1691	31.557	-2.010	13.567	1.00	23.41
7	MOTA	1991	CZ2	TRP	1691	31.617	-0.011	15.097	1.00	25.00
I	MOTA	1992	CZ3	TRP	1691	29.398	0.851	15.573	1.00	26.78
7	MOTA	1993	CH2	TRP	1691	30.802	0.900	15.719	1.00	27.78
7	MOTA	1994	C	TRP	1691	26.947	-3.088	15.012	1.00	28.70
I	MOTA	1995	O	TRP	1691	27.708	-3.245	15.974	1.00	29.56
7	MOTA	1996	N	GLU	1692	25.808	-2.400	15.104	1.00	29.51
Į	MOTA	1998	CA	GLU	1692	25.349	-1.817	16.371	1.00	27.55
7	MOTA	1999	CB	GLU	1692	24.120	-0.935	16.171	1.00	28.35
	MOTA	2000	CG	GLU	1692	24.273	0.221	15.219	1.00	24.70
7	MOTA	2001	CD	GLU	1692	22.982	0.989	15.100	1.00	25.44
7	MOTA	2002	OE1	GLU	1692	22.224	0.744	14.148	1.00	24.34
7	MOTA	2003	OE2	GLU	1692	22.696	1.816	15.982	1.00	27.57
P	MOTA	2004	C	GLU	1692	24.958	-2.918	17.352	1.00	28.74
A	MOTA	2005	0	GLU	1692	25.099	-2.753	18.557	1.00	28.76
	MOT	2006	N	ILE	1693	24.421	-4.023	16.844	1.00	29.23
	MOT	2008	CA	ILE	1693	24.027	-5.125	17.712	1.00	27.48
	MOTA	2009	CB	ILE	1693	23.205	-6.226	16.944	1.00	28.80
	MOT	2010	CG2	ILE	1693	22.983	-7.469	17.842	1.00	22.98
	TOM	2011	CG1	ILE	1693	21.840	-5.658	16.508	1.00	27.36
	MOT	2012	CD1	ILE	1693	21.005	-6.585	15.635	1.00	24.84
	TOM	2013	C	ILE	1693	25.259	-5.750	18.357	1.00	27.27
	TOM	2014	0	ILE	1693	25.320	-5.902	19.575	1.00	28.15
	TOM	2015	N	PHE	1694	26.273	-6.043	17.552	1.00	27.83
		2017	CA	PHE	1694	27.473	-6.677	18.095	1.00	29.88
	TOM	2018	CB	PHE	1694	28.143	-7.525	17.011	1.00	28.66
	TOM	2019	CG	PHE	1694	27.223	-8.574	16.463	1.00	29.92
	TOM	2020	CD1	PHE	1694	26.628	-8.424	15.220	1.00	30.20
	MOT	2021	CD2	PHE	1694	26.809	-9.630	17.269	1.00	30.81
		2022	CE1	PHE	1694	25.625	-9.294	14.801	1.00	32.42
	TOM TOM	2023 2024	CE2 CZ	PHE PHE	1694 1694	25.805	-10.508	16.857	1.00	32.30
			C	PHE	1694	25.210 28.429	-10.337	15.628	1.00	31.13
		2025	0	PHE	1694	29.376	-5.784 -6.273	18.890	1.00	31.07
			N	THR	1695	28.157	-4.480	19.509 18.897	1.00	33.16 29.20
		2029	CA	THR	1695	28.934	-3.532		1.00	
		2030	CB	THR	1695	29.412	-2.333	19.670 18.823	1.00	27.38
			OG1	THR	1695	28.287	-1.652	18.274	1.00	24.77 26.27
			CG2	THR	1695	30.305	-2.800	17.706	1.00	
			C	THR	1695	28.053	-3.034	20.822	1.00	20.18 29.84
			0	THR	1695	28.430	-2.103	21.548	1.00	32.77
				LEU	1696	26.898	-3.687	20.988	1.00	
				LEU	1696	25.915	-3.867	22.029	1.00	28.52
				LEU	1696	26.356	-3.886	23.394	1.00	32.50
				LEU	1696	26.658	-5.379	23.476	1.00	33.24
				LEU	1696	27.205	-5.717	24.849	1.00	34.15
				LEU	1696	25.398	-6.150	23.191	1.00	37.24
~		2032	<b>-D2</b>		2000	23.330	-0.130	43.131	1.00	31.24



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ATC		–	LE		25.553	-1.88	8 22.13	1 1.00	26.98
ATC	_		LE		25.579				
ATC			GL		25.148				
ATC					24.767	0.074			
ATO			GL		25.927	0.962			
ATO			GL		25.957	2.132			
ATO		_	GL		26.888	0.416			
ATO ATO					28.031	1.212			
ATO		_	GL.		27.651	2.301			
		_	GL.		26.669	2.177			· <b>-</b> ·
ATO:			SEI		28.418	3.380			
			SEI		28.168	4.491			
ATO! ATO!			SE		28.438	5.810			31.77
ATOM			SEF		28.575	6.919			38.42
ATOM		_	SER		29.093	4.350			27.98
ATOM			SER		30.299	4.310	16.529	1.00	28.18
ATOM			PRO		28.537	4.240	15.153	1.00	29.62
ATOM			PRO		27.104	4.259	14.794	1.00	31.22
ATOM			PRO		29.381	4.107	13.958	1.00	28.95
ATOM			PRO		28.356	4.003	12.807	1.00	27.21
ATOM			PRO		27.095	3.556	13.460	1.00	29.33
ATOM			PRO		30.205	5.379	13.773	1.00	28.78
ATOM		-	PRO		29.737	6.469	14.110	1.00	30.04
ATOM		• •	TYR		31.426	5.239	13.264	1.00	28.35
ATOM			TYR		32.296	6.390	12.987	1.00	30.77
ATOM	•	CG	TYR	1701	31.921	6.987	11.615	1.00	31.67
ATOM	2075		TYR	1701	32.060	6.037	10.454	1.00	34.61
ATOM	2076	CE1	TYR		30.952	5.673	9.686	1.00	38.26
ATOM	2077	CD2	TYR TYR	1701	31.083	4.806	8.587	1.00	40.99
ATOM	2078	CE2	TYR	1701	33.301	5.520	10.106	1.00	38.16
ATOM	2079	CZ	TYR	1701	33.449	4.662	9.020	1.00	41.04
ATOM	2080	ОН	TYR	1701	32.343	4.312	8.263	1.00	43.11
ATOM	2082	C	TYR	1701 1701	32.531	3.478	7.181	1.00	49.53
ATOM	2083	Ö	TYR	1701	32.305	7.532	14.029	1.00	31.41
ATOM	2084	N	PRO	1701	32.026	8.689	13.698	1.00	33.59
ATOM	2085	CD	PRO	1702	32.635	7.230	15.296	1.00	30.92
ATOM	2086	CA	PRO	1702	32.998	5.938	15.888	1.00	32.30
ATOM	2087	CB	PRO	1702	32.656 33.123	8.283	16.314	1.00	30.05
ATOM	2088	CG	PRO	1702	32.676	7.548	17.561	1.00	27.77
ATOM	2089	C	PRO	1702	33.659	6.174	17.338	1.00	32.34
MOTA	2090	0	PRO	1702	34.769	9.366	15.944	1.00	31.42
ATOM	2091	N	GLY	1703	33.257	9.055	15.513	1.00	30.95
ATOM	2093	CA	GLY	1703	34.122	10.627	16.117		31.30
ATOM	2094	С	GLY	1703	34.172	11.751	15.817		29.66
MOTA	2095	0	GLY	1703	34.752	12.138			31.00
MOTA	2096	N	VAL	1704	33.551	13.165	13.999		30.69
ATOM	2098	CA	VAL	1704	33.551	11.331	13.491		31.11
MOTA	2099	CB	VAL	1704	33.539	11.610	12.059		29.88
ATOM	2100	CG1	VAL	1704	33.585	10.310			28.41
ATOM	2101	CG2	VAL	1704	34.702	10.624			26.24
MOTA	2102	C	VAL	1704	32.396				24.10
MOTA	2103	0	VAL	1704	31.224				30.80
MOTA	2104	N	PRO	1705	32.718				32.50
					/10	13.705	11.104	1.00	30.86

ATOM	2105	CD	PRO	1705	34.039	14.350	11.077	1.00	30.59
ATOM	2106	CA	PRO	1705	31.682	14.625	10.645	1.00	31.47
ATOM	2107	CB	PRO	1705	32.400	15.971	10.680	1.00	32.75
ATOM	2108	CG	PRO	1705	33.774	15.607	10.289	1.00	32.59
ATOM	2109	C	PRO	1705	31.258	14.264	9.239	1.00	32.19
ATOM	2110	0	PRO	1705	31.974	13.536	8.549	1.00	33.91
MOTA	2111	N	VAL	1706	30.124	14.814	8.806	1.00	32.57
ATOM	2113	CA	VAL	1706	29.560	14.576	7.474	1.00	31.80
ATOM	2114	CB	VAL	1706	28.483	15.632	7.172	1.00	34.66
ATOM	2115	CG1	VAL	1706	28.022	15.538	5.738	1.00	39.06
ATOM	2116	CG2	VAL	1706	27.309	15.455	8.106	1.00	36.62
ATOM	2117	С	VAL	1706	30.578	14.560	6.320	1.00	31.58
ATOM	2118	0	VAL	1706	30682	13.585	5.570	1.00	32.35
ATOM	2119	N	GLU	1707	31.326	15.649	6.189	1.00	31.46
ATOM	2121	CA	GLU	1707	32.329	15.788	5.139	1.00	31.68
ATOM	2122	CB	GLU	1707	33.021	17.148	5.267	1.00	32.59
ATOM	2123	C	GLU	1707	33.381	14.678	5.114	1.00	32.23
ATOM	2124	0	GLU	1707	33.740	14.183	4.050	1.00	33.47
ATOM	2125	N	GLU	1708	33.902	14.316	6.279	1.00	32.90
ATOM	2127	CA	GLU	1708	34.909	13.268	6.352	1.00	33.86
ATOM ATOM	2128	CB CG	GLU	1708	35.570	13.244	7.730	1.00	38.54
ATOM	2129 2130	CD	GLU GLU	1708		14.575	8.165	1.00	47.63
ATOM	2130	OE1	GLU	1708	37.442	14.962	7.383	1.00	58.35
ATOM	2132	OE2	GLU	1708 1708	38.117	14.067	6.816	1.00	62.88
ATOM	2132	C C	GLU	1708	37.770	16.176	7.355	1.00	64.79
ATOM	2134	0	GLU	1708	34.276 34.927	11.921 11.038	6.043	1.00	33.56
ATOM	2135	N	LEU	1709	32.997	11.774	5.489 6.374	1.00	34.18
ATOM	2137	CA	LEU	1709	32.285	10.532	6.108	1.00 1.00	32.91
ATOM	2138	CB	LEU	1709	30.862	10.563	6.685	1.00	33.83 32.28
ATOM	2139	CG	LEU	1709	30.015	9.363	6.231	1.00	32.92
ATOM	2140	CD1	LEU	1709	30.541	8.071	6.853	1.00	28.37
ATOM	2141	CD2	LEU	1709	28.563	9.580	6.568	1.00	31.90
ATOM	2142	C'	LEU	1709	32.222	10.283	4.60€	1.00	34.15
MOTA	2143	0	LEU	1709	32.412	9.152	4.156	1.00	34.75
MOTA	2144	N	PHE	1710	31.918	11.332	3.844	1.00	33.83
ATOM	2146	CA	PHE	1710	31.828	11.248	2.388	1.00	32.90
MOTA	2147	CB	PHE	1710	31.531	12.622	1.787	1.00	34.85
MOTA	2148	CG	PHE	1710	30.162	13.132	2.082	1.00	38.60
ATOM	2149	CD1	PHE	1710	29.150	12.268	2.469	1.00	43.69
MOTA	2150	CD2	PHE	1710	29.882	14.480	1.984	1.00	45.10
MOTA	2151	CE1	PHE	1710	27.873	12.742	2.764	1.00	46.23
ATOM	2152	CE2	PHE	1710	28.611	14.966	2.274	1.00	48.15
MOTA	2153	CZ	PHE	1710	27.603	14.086	2.670	1.00	46.90
ATOM	2154	С	PHE	1710	33.131	10.739	1.803	1.00	31.84
MOTA	2155	0	PHE	1710	33.134	9.931	0.877	1.00	29.97
ATOM	2156	N	LYS	1711	34.231	11.224	2.373	1.00	32.45
MOTA	2158	CA	LYS	1711	35.582	10.860	1.947	1.00	34.53
ATOM	2159	CB	LYS	1711	36.588	11.755	2.675	1.00	36.17
ATOM	2160	CG	LYS	1711	38.008	11.669	2.182	1.00	41.07
ATOM	2161	CD	LYS	1711	38.912	12.582	3.001	1.00	46.23
ATOM	2162	CE	LYS	1711	40.311	12.648	2.418	1.00	51.79
ATOM	2163	NZ	LYS	1711	41.036	11.360	2.556	1.00	57.27
ATOM	2167	С	LYS	1711	35.867	9.375	2.215	1.00	33.82

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					23	6		
MOT	2168	0	LYS	1711	36.451	8.688	1.376	1 00
MOT	2169	N	LEU	1712	35.439	8.885		
MOT	2171	CA	LEU	1712	35.618	7.477	3.382	
TOM	2172	CD	TEST			7.3//	3.754	1.00

A' 33.20 A. O 34.52 A' 0 33.25 ATOM LEU 1712 35.094 7.211 5.189 1.00 30.99 ATOM 2173 CG LEU 1712 35.746 7.917 6.393 1.00 29.71 **ATOM** 2174 CD1 LEU 1712 35.047 7.552 7.678 1.00 24.11 **ATOM** 2175 CD<sub>2</sub> LEU 1712 37.208 7.552 6.497 1.00 32.21 MOTA 2176 C LEU 1712 34.833 6.631 2.744 1.00 32.16 ATOM 2177 0 LEU 1712 35.378 5.732 2.109 1.00 ATOM 32.77 2178 N LEU 1713 33.562 6.967 2.563 1.00 31.72 MOTA 2180 CA LEU 1713 32.700 6.259 1.637 1.00 33.60 MOTA 2181 CB LEU 1713 31.299 6.879 1.619 1.00 **ATOM** 36.57 2182 CG LEU 1713 30.522 6.711 2.930 1.00 37.60 ATOM 2183 CD1 LEU 1713 29.284 7.575 2.927 1.00 35.03 MOTA 2184 CD2 LEU 1713 30.182 5.246 3.157 1.00 33.22 ATOM 2185 С LEU 1713 33.285 6.248 0.236 1.00 35.33 ATOM 2186 0 LEU 1713 33.318 5.203 -0.407 1.00 36.00 ATOM 2187 N LYS 1714 33.741 7.405 -0.234 1.00 36.24 MOTA 2189 CA LYS 1714 34.331 7.501 -1.566 1.00 36.35 MOTA 2190 CB LYS 1714 34.707 8.946 -1.900 1.00 35.82 ATOM 2191 CG LYS 1714 33.520 9.837 -2.168 1.00 37.23 MOTA 2192 CD LYS 1714 32.712 9.324 -3.337 1.00 40.53 MOTA 2193 CE LYS 1714 31.506 10.198 -3.600 1.00 44.51 ATOM 2194 NZ LYS 1714 30.747 9.724 -4.804 1.00 50.76 ATOM 2198 C LYS 1714 35.559 6.613 -1.701 1.00 37.60 ATOM 2199 О LYS 1714 35.808 6.039 -2.764 1.00 40.82 MOTA 2200 N GLU 1715 36.299 -0.615 6.452 1.00 35.61 ATOM 2202 CA GLU 1715 37.496 5.630 ~0.658 1.00 34.65 MOTA 2203 CB GLU 1715 38.517 6.188 0.320 1 00 37.83 MOTA 2204 CG GLU 1715 38.897 7.613 -0.036 1.00 42.28 ATOM 2205 CD GLU 1715 39.634 8.342 1.061 1.00 45.64 MOTA 2206 OE1 GLU 1715 39.928 7.726 2.114 1.00 43.09 ATOM 2207 OE2 GLU 1715 39.918 9.544 0.853 1.00 47.56 MOTA 2208 С GLU 1715 37.244 4.145 ~0.419 1.00 32.94 MOTA 2209 O GLU 1715 38.177 3.348 -0.419 1.00 33.31 MOTA 2210 N GLY 1716 35.983 3.779 -0.213 1.00 29.12 MOTA 2212 CA GLY 1716 35.634 2.391 0.004 1.00 26.02 MOTA 2213 С GLY 1716 35.946 1.895 1.396 1.00 29.60 **ATOM** 2214 0 GLY 1716 36.223 0.715 1.588 1.00 29.81 MOTA 2215 N HIS 1717 35.879 2.783 2.379 1.00 29.97 **ATOM** 2217 CA HIS 1717 36.158 2.409 3.763 1.00 30.78 MOTA 2218 CB HIS 1717 36.369 3.659 4.623 1.00 33.25 MOTA 2219 CG HIS 1717 36.653 3.360 6.067 1.00 34.70 MOTA 2220 CD2 HIS 1717 37.820 3.155 6.715 1.00 32.77 MOTA 2221 ND1 HIS 1717 35.656 3.219 7.010 1.00 36.90 MOTA 2223 CE1 HIS 1717 36.200 2.932 8.180 1.00 35.87 ATOM 2224 NE2 HIS 1717 37.513 2.887 8.027 1.00 31.93 ATOM 2226 C HIS 1717 35.035 1.577 4.375 1.00 29.63 ATOM 2227 0 HIS 1717 33.861 1.847 4.133 1.00 30.82 MOTA 2228 N ARG 1718 35.406 0.600 5.201 1.00 27.92 **ATOM** 2230 CA ARG 1718 34.436 -0.258 5.878 1.00 27.30 **ATOM** 2231 CB ARG 1718 34.379 -1.641 5.236 1.00 24.10 MOTA 2232 CG ARG 1718 33.939 -1.655 3.789 1.00 26.52 MOTA 2233 CD ARG 1718 32.469 -1.288 3.627 1.00 26.96



	ATOM	2234	NE	ARG	1718	32.020	-1.374	2.232	1.00	24.41
	ATOM	2236	CZ	ARG	1718	32.090	-0.377	1.352	1.00	25.51
	MOTA	2237	NH1	ARG	1718	32.611	0.801	1.706	1.00	23.61
	MOTA	2240	NH2	ARG	1718	31.553	-0.521	0.149	1.00	21.28
	ATOM	2243	C	ARG	1718	34.881	-0.384	7.330	1.00	28.81
	MOTA	2244	0	ARG	1718	36.080	-0.425	7.611	1.00	29.77
	ATOM	2245	N	MET	1719	33.920	-0.377	8.250	1.00	30.40
	ATOM	2247	CA	MET	1719	34.215	-0.485	9.673	1.00	30.62
	MOTA	2248	CB	MET	1719	32.942	-0.339	10.497	1.00	28.91
	MOTA	2249	CG	MET	1719	32.235	1.003	10.316	1.00	30.85
	ATOM	2250	SD	MET	1719	30.829	1.237	11.432	1.00	33.27
	ATOM	2251	CE	MET	1719	29.521	0.416	10.561	1.00	31.81
•	ATOM	2252	C	MET	1719	34.900	-1.793	10.005	1.00	31.32
	ATOM	2253	0	MET	1719	34.755	-2.769	9.278	1.00	31.47
	ATOM	2254	N	ASP	1720	35.651	-1.799	11.103	1.00	33.78
	ATOM	2256	CA	ASP	1720	36.387	-2.983	11.550	1.00	33.45
	MOTA	2257	CB	ASP	1720	37.478	-2.580	12.546	1.00	36.99
	ATOM	2258	CG	ASP	1720	38.585	-1.762	11.908	1.00	41.56
	ATOM	2259	OD1	ASP	1720	38.403	-1.339	10.742	1.00	48.43
	MOTA	2260	OD2	ASP	1720	39.634	-1.546	12.568	1.00	40.99
	MOTA	2261	C	ASP	1720	35.473	-4.001	12.211	1.00	32.12
	ATOM	2262	0	ASP	1720	34.381	-3.657	12.668	1.00	30.89
	ATOM	2263	N	LYS	1721	35.944	-5.241	12.328	1.00	31.82
	MOTA	2265	CA	LYS	1721	35.127	-6.270	12.953	1.00	31.71
	ATOM	2266	CB	LYS	1721	35.691	-7.679	12.747	1.00	32.34
	MOTA	2267	CG	LYS	1721	34.762	-8.738	13.344	1.00	34.85
	ATOM	2268	CD	LYS	1721	35.111	-10.155	12.961	1.00	37.39
	MOTA	2269	CE	LYS	1721	36.266	-10.674	13.765	1.00	41.42
	ATOM	2270	ΝZ	LYS	1721	36.348	-12.154	13.635	1.00	4655
	ATOM	2274	C	LYS	1721	35.007	-6.018	14.430	1.00	33.40
	MOTA	2275	0	LYS	1721	36.017	-5.879	15.121	1.00	34.26
	ATOM	2276	N	PRO	1722	33.768	-5.924	14.934	1.00	34.26
	ATOM	2277	CD	PRO	1722	32.494	-6.002	14.203	1.00	32.16
	ATOM	2278	CA	PRO	1722	33.546	-5.692	16.362	1.00	35.84
	ATOM	2279	. CB	PRO	1722	32.027	-5.682	16.473	1.00	35.35
	MOTA	2280	CG	PRO	1722	31.575	~5.255	15.108	1.00	35.35
	ATOM	2281	С	PRO	1722	34.105	-6.904	17.099	1.00	40.41
	ATOM	2282	0	PRO	1722	34.010	-8.038	16.607	1.00	41.14
	MOTA	2283	N	SER	1723	34.739	-6.680	18.240	1.00	43.60
	ATOM	2285	CA	SER	1723	35.260	-7.808	18.999	1.00	45.51
	ATOM	2286	CB	SER	1723	36.078	-7.324	20.191	1.00	45.30
	ATOM	2287	OG	SER	1723	35.384	-6.300	20.879	1.00	49.62
	MOTA	2289	C	SER	1723	34.031	-8.589	19.460	1.00	46.39
	ATOM	2290	0	SER	1723	32.939	-8.028	19.614	1.00	45.16
	ATOM	2291	N	ASN	1724	34.199	-9.891	19.631	1.00	48.53
	MOTA	2293	CA	ASN	1724	33.088	-10.723	20.065	1.00	51.13
	MOTA	2294	CB	ASN	1724	32.509	-10.194	21.390	1.00	56.87
	ATOM	2295	CG	ASN	1724	33.595	-9.892	22.427	1.00	61.65
	ATOM	2296	OD1	ASN	1724	34.503	-10.702	22.649	1.00	63.73
	MOTA	2297	ND2	ASN	1724	33.526	-8.713	23.039	1.00	64.64
	MOTA	2300	С	ASN	1724	32.034	-10.743	18.941	1.00	48.83
	MOTA	2301	0	ASN	1724	30.846	-10.534	19.145	1.00	50.50
	ATOM	2302	N	CYS	1725	32.511	-10.977	17.734	1.00	45.23
	ATOM	2304	CA	CYS	1725	31.654	-11.056	16.570	1.00	42.33



	TOM					31.57	0 -9.702	15.85	4 1.00	2 42 40
	TOM					30.71				
	TOM		_	CY		32.38	3 -12.077			
	TOM	230		CY		33.60	1 -12.004			· · · · •
	MOT	230		TH	· -	31.66	4 -13.090			
	MOT	231			· -	32.27	5 -14.139	14.459		
	MOT	231				31.30	L -15.326	14.326		
	MO	231				30.071	-14.904	13.711		
	MO	231				30.981	~15.861	15.696		
	MO	2316	_	THI		32.720	-13.629	13.092		
	MO'	2311	_	THE		32.257	-12.593	12.643		
AT		2318		ASI		33.643	-14.315	12.434		-
AT		2320		ASI		34.050		1.1.114		
AT		2321		ASN		35.198	-14.680	10.541		34.97
AT		2322	_	ASN		36.540	-14.271	11.103	1.00	39.89
AT		2323				37.044		10.826	1.00	45.37
ATO		2324				37.125	-15.141	11.909	1.00	48.43
ATO		2327	_	ASN		32.846	-13.947	10.192	1.60	45.88 33.97
ATO		2328		ASN		32.646	-13.088	9.341	1.00	35.97
ATO		2329		GLU		32.024	-14.973	10.414	1.00	31.69
ATO		2331	CA	GLU		30.814	-15.210	9.620	1 00	30.27
ATC		2332 2333	CB	GLU		30.141	-16.493	10.083	1.00	32.53
ATC		2334	C.G	GLU	1728	28.932	-16.878	9.273	1.00	32.81
ATC		2335	CD	GLU	1728	28.353	-18.190	9.711	1.00	36.43
ATO		2336	OE1	GLU	1728	28.339	-18.466	10.932	1.00	36.75
ATO		2337	OE2	GLU	1728	27.908	-18.945	8.829	1.00	41.92
ATO		2338	С 0	GLU	1728	29.814	-14.049	9 681	1.00	28.70
ATO		2339	N	GLU	1728	29.234	-13.655	8.660	1.00	28.51
ATO		2341	CA	LEU	1729	29.594	-13.517	10.880	1.00	26.77
ATO		2342	CB	LEU	1729	28.687	-12.393	11.040	1.00	26.80
ATO		2343	CG	LEU LEU	1729	28.228	-12.274	12.490	1.00	27.91
ATO		2344	CD1	LEU	1729	27.233	-13.355	12.913	1.00	30.71
ATO	M	2345	CD2	LEU	1729	27.095	-13.345	14.428	1.00	35.79
ATO		2346	C	LEU	1729	25.885	-13.141	12.253	1.00	25.70
ATO		2347	o	LEU	1729 1729	29.319	-11.089	10.540	1.00	27.06
ATON		2348	N	TYR	1730	28.610	-10.177	10.126	1.00	30.27
ATON		2350	CA	TYR	1730	30.650		10.549	1.00	27.03
ATOM		2351	СВ	TYR	1730	31.328		10.039	1.00	26.21
ATOM	1 :	2352	CG	TYR	1730	32.792 33.538		10.474	1.00	25.31
ATOM	1 :	2353	CD1	TYR	1730	33.012	-8.553	9.982	1.00	24.89
ATOM	1 :	2354	CE1	TYR	1730	33.655	-7.270	10.169	1.00	23.59
ATOM	1 2	2355	CD2	TYR	1730	34.739	-6.148	9.665		24.74
ATOM	1 2	2356	CE2	TYR	1730	35.399	-8.675	9.285		22.11
ATOM	1 2	357	CZ	TYR	1730	34.853	-7.560	8.775		22.32
ATOM	1 2	358	ОН	TYR	1730	35.484	-6.295		1.00	26.07
ATOM	2	360	C	TYR	1730	31.227	-5.181	8.418		22.70
ATOM	2	361	0	TYR	1730	30.960	-9.878		1.00	27.71
ATOM	2	362	N	MET	1731		-8.875		1.00	28.05
MOTA		364	CA	MET	1731	31.409 31.306	-11.081			27.92
ATOM	2	365	CB	MET	1731		-11.355			28.89
ATOM		366	CG	MET	1731	31.506 31.068	-12.853			35.84
MOTA		367	SD	MET	1731	31.347	-13.379			45.50
MOTA		368	CE	MET	1731		-15.167 <sub>8</sub>		1.00	56.40
				_		22.100	-15.263	3.217	1.00	66.88
CCC		_								

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MOTA	2369	С	MET	1731	29.916	-10.928	6.102	1.00	27.79
ATOM	2370	0	MET	1731	29.755	-10.345	5.041	1.00	30.68
ATOM	2371	N	MET	1732	28.915	-11.203	6.932	1.00	28.02
MOTA	2373	CA	MET	1732	27.546	-10.804	6.639	1.00	25.74
MOTA	2374	CB	MET	1732	26.598	-11.317	7.718	1.00	24.94
MOTA	2375	CG	MET	1732	25.153	-10.911	7.492	1.00	22.96
MOTA	2376	SD	MET	1732	24.008	-11.593	8.684	1.00	24.39
MOTA	2377	CE	MET	1732	23.798	-13.272	8.002	1.00	18.04
ATOM	2378	C	MET	1732	27.470	-9.273	6.559	1.00	25.81
ATOM	2379	0	MET	1732	26.889	-8.729	5.620	1.00	26.85
MOTA	2380	N	MET	1733	28.068	-8.587	7.53.7	1.00	24.84
ATOM	2382	CA	MET	1733	28.092	-7.124	7.545	1.00	25.27
MOTA	2383	CB	MET	1733	28.931	-6.6.00	9.700	1.00	25.97
ATOM	2384	CG	MET	1733	28.342	-6.769	10.058	1.00	28.69
MOTA	2385	SD	MET	1733	29.456	-6.094	11.295	1.00	29.06
ATOM	2386	CE	MET	1733	28.927	-7.051	12.693	1.00	28.07
ATOM	2387	С	MET	1733	28.741	-6.628	6.270	1.00	26.97
ATOM	2388	0	MET	1733	28.192	-5.771	5.581	1.00	28.37
ATOM	2389	N	ARG	1734	29.922	-7.160	5.966	1.00	28.77
ATOM	2391	CA	ARG	1734	30.664	-6. <b>7</b> 75	4.762	1.00	29.66
ATOM	2392	CB	ARG	1734	32.027	-7.482	4.716	1.00	29.05
ATOM	2393	CG	ARG	1734	32.968	-7.109	5.866	1.00	25.00
ATOM	2394	CD	ARG	1734	33.247	-5.621	5.882	1.00	29.27
MOTA	2395	NE	ARG	1734	33.911	-5.210	4.647	1.00	35.43
MOTA	2397	CZ	ARG	1734	35.233	-5.220	4.466	1.00	38.24
ATOM	2398	NH1	ARG	1734	36.054	-5.601	5.445	1.00	36.47
ATOM	2401	NH2	ARG	1734	35.732	-4.907	3.277	1.00	38.57
ATOM	2404	C	ARG	1734	29.859	-7.034	3.478	1.00	29.57
MOTA	2405	0	ARG	1734	29.920	-6.242	2.538	1.00	29.55
MOTA	2406	N	ASP	1735	29.095	-8.124	3.448	1.00	28.07
MOTA	2408	CA	ASP	1735	28.259	-8.423	2.287	1.00	27.96
MOTA	2409	CB	ASP	1735	27.634	-9.813	2.408	1.00	28.60
ATOM	2410	CG	ASP	1735	28.664	-10.926	2.283	1.00	31.34
MOTA	2411	OD1	ASP	1735	29.785	-10.660	1.798	1.00	31.12
ATOM	2412	OD2	ASP	1735	28.356	-12.068	2.687	1.00	36.07
MOTA	2413	С	ASP	1735	27.159	-7.368	2.155	1.00	27.24
MOTA	2414	0	ASP	1735	26.846	-6.932	1.050	1.00	25.79
MOTA	2415	N	CYS	1736	26.590	-6.951	3.288	1.00	26.53
MOTA	2417	CA	CYS	1736	25.547	-5.930	3.314	1.00	24.35
MOTA	2418	CB	CYS	1736	24.968	-5.765	4.731	1.00	22.01
ATOM	2419	SG	CYS	1736	23.885	-7.101	5.281	1.00	21.52
MOTA	2420	C	CYS	1736	26.119	-4.595	2.847	1.00	24.26
MOTA	2421	0	CYS	1 <b>7</b> 36	25.386	-3.725	2.368	1.00	24.19
MOTA	2422	N	TRP	1737	27.432	-4.437	3.002	1.00	22.94
ATOM	2424	CA	TRP	1737	28.104	-3.210	2.605	1.00	21.91
ATOM	2425	CB	TRP	1737	29.146	-2.820	3.640	1.00	19.26
MOTA	2426	CG	TRP	1737	28.572	-2.493	4.947	1.00	20.89
ATOM	2427	CD2	TRP	1737	29.226	-2.602	6.212	1.00	23.33
ATOM	2428	CE2	TRP	1737	28.315	-2.159	7.196	1.00	21.59
ATOM	2429	CE3	TRP	1737	30.506	-3.026	6.614	1.00	25.00
ATOM	2430	CD1	TRP	1737	27.319	-2.012	5.201	1.00	19.90
ATOM	2431	NE1	TRP	1737	27.158	-1.807	6.551	1.00	20.77
ATOM	2433	CZ2	TRP	1737	28.641	-2.127	8.563	1.00	19.89
ATOM	2434	CZ3	TRP	1737	30.825	-2.993	7.971	1.00	21.23



A TON									
ATON					29.896	-2.543	8.927	1.00	21.09
ATOM			TRI	1737	28.758				
ATOM			TRE	1737	29.653				
ATOM			HIS	1738	28.315	-4.185			
ATOM			HIS	1738	28.877	-4.287			
ATOM			HIS	1738	28.243				
ATOM			HIS	1738	29.131				
ATOM		CD2	HIS	1738	29.595				
ATOM		ND1	HIS		29.681				
ATOM		CE1	HIS	1738	30.436				
ATOM		NE2	HIS	1738	30.409			1.00	
ATOM	2449	C	HIS	1738	28.716			1.00	
ATOM	2450	0	HIS	1738	27.675			1.00	
ATOM	2451	N	ALA	1739	29.802	-2.314		1.00	23.96
ATOM	2453	CA	ALA	1739	29.825	-2.564	-2.362	1.00	26.27
ATOM	2454	CB	ALA	1739	31.186	-1.346	-3.158	1.00	25.46
ATOM	2455	С	ALA	1739	28.754	-1.180	-3.789	1.00	25.70
ATOM	2456	0	ALA	1739		-1.443	-4.233	1.00	26.18
ATOM	2457	N	VAL	1740	28.116	-0.455	-4.574	1.00	29.14
ATOM	2459	CA	VAL	1740	28.570	-2.643	-4.774	1.00	25.71
ATOM	2460	СВ	VAL		27.560	-2.875	-5.802	1.00	26.12
ATOM	2461	CG1	VAL	1740	28.063	-3.841	-6.903	1.00	25.99
ATOM	2462	CG2	VAL	1740	27.102	~3.832	-8.090	1.00	23.37
ATOM	2463	C	VAL	1740	29.450	-3.440	-7.349	1.00	22.07
ATOM	2464	0	VAL	1740	26.247	-3.400	-5.191	1.00	25.43
ATOM	2465	N	PRO	1740	26.186	-4.550	-4.704	1.00	24.93
ATOM	2466	CD		1741	25.170	-2.585	-5.265	1.00	24.20
ATOM	2467	CA	PRO	1741	25.151	÷1.277	-5.953	1.00	18.88
ATOM	2468	CB	PRO	1741	23.838	-2.914	-4.734	1.00	25.28
ATOM	2469		PRO	1741	22.953	-1.788	-5.294	1.00	22.75
ATOM	2470	CG	PRO	1741	23.903	-0.632	-5.398	1.00	20.99
ATOM	2470	C	PRO	1741	23.299	-4.296	-5.128	1.00	25.84
ATOM		C	PRO	1741	22.787	-5.036	-4.280	1.00	25.99
ATOM	2472	N .	SER	1742	23.425	-4.642	-6.407	1.00	26.48
ATOM	2474	CA	SER	1742	22.942	<b>-5.9</b> 19	-6.930	1.00	25.19
ATOM	2475	CB	SER	1742	23.151	-5.992	-8.440	1.00	25.68
ATOM	2476	OG	SER	1742	24.530	-5.943	-8.769	1.00	27.46
ATOM	2478	C	SER	1742	23.644	-7.100	-6.289	1.00	25.24
	2479	0	SER	1742	23.124	-8.218	-6.300	1.00	26.09
ATOM ATOM	2480	N	GLN	1743	24.826	-6.851	-5.731	1.00	23.88
	2482	CA	GLN	1743	25.590	-7.917	-5.118	1.00	24.44
ATOM	2483	CB	GLN	1743	27.069	-7.733	-5.437	1.00	27.26
ATOM	2484	CG	GLN	1743	27.344	-7.784	-6.940	1.00	27.39
ATOM	2485	CD	GLN	1743	26.803	-9.047	-7.581	1.00	26.46
ATOM	2486	OE1	GLN	1743	27.325	-10.136	-7.339	1.00	
ATOM	2487	NE2	GLN	1743	25.760	-8.914	-8.393	1.00	25.80
ATOM	2490	C	GLN	1743	25.348	-8.151	-3.633		27.42
ATOM	2491	0	GLN	1743	25.810	-9.147	-3.083	1.00	23.20
ATOM	2492	N	ARG	1744	24.628	-7.243	-2.984	1.00	22.90
	2494		ARG	1744	24.318	-7.398		1.00	22.15
ATOM	2495		ARG	1744	23.767	-6.088	-1.568	1.00	21.23
ATOM	2496			1744	24.705			1.00	19.01
	2497			1744	24.091	-4.916		1.00	17.27
				1744	24.914	-3.605 -3.403		1.00	14.79
				1744		-2.493		1.00	19.72
			- 41.0	<u> </u>	24.482	-1.258	-1.391	1.00	19.23

ATOM	2501	NHl	ARG	1744	23.201	-0.931	-1.201	1.00	15.90
ATOM	2504	NH2	ARG	1744	25.343	-0.343	-1.821	1.00	19.43
ATOM	2507	С	ARG	1744	23.259	-8.496	-1.438	1.00	21.95
ATOM	2508	0	ARG	1744	22.585	-8.827	-2.415	1.00	25.34
MOTA	2509	N	PRO	1745	23.213	-9.184	-0.292	1.00	20.82
ATOM	2510	CD	PRO	1745	24.191	-9.219	0.804	1.00	21.25
ATOM	2511	CA	PRO	1745	22.204	-10.229	-0.127	1.00	21.39
ATOM	2512	СВ	PRO	1745	22.687	-10.980	1.117	1.00	21.69
ATOM	2513	CG	PRO	1745	23.418	-9.916	1.886	1.00	22.62
MOTA	2514	C	PRO	1745	20.833	-9.585	0.102	1.00	22.15
ATOM	2515	0	PRO	1745	20.739	-8.402	0.426	1.00	23.29
MOTA	2516	N	THR	1746	19.771	-10.349	-0.109	1.00	20.93
ATOM	2518	CA	THR	1746	18.440	-9.827	0.107	1.00	19.90
ATOM	2519	CB	THR	1746	17.391	-10.554	-0.783	1.00	20.21
ATOM ATOM	2520 2522	OG1 CG2	THR	1746	17.484	-11.974	-0.584	1.00	22.03
ATOM	2522	CG2	THR THR	1746 1746	17.609 18.112	-10.242	-2.255	1.00	20.82
ATOM	2523	0	THR	1746	18.112	-10.095	1.557	1.00	19.77
ATOM	2525	И	PHE	1747		-10.823	2.228	1.00	19.19
ATOM	2527	CA	PHE	1747	17.010 16.582	-9.526 -9.770	2.045	1.00	23.46
ATOM	2528	CB	PHE	1747	15.473	-8.794	3.422 3.827	1.00	21.64
ATOM	2529	CG	PHE	1747	15.987	-7.445	4.262	1.00	18.69 17.45
ATOM	2530	CD1	PHE	1747	16.757	-7.317	5.417	1.00	17.45
ATOM	2531	CD2	PHE	1747	15.712	-6.303	3.516	1.00	15.37
ATOM	2532	CE1	PHE	1747	17.242	-6.073	5.819	1.00	16.17
ATOM	2533	CE2	PHE	1747	16.189	-5.056	3.907	1.00	14.53
ATOM	2534	CZ	PHE	1747	16.959	-4.941	5.065	1.00	16.98
ATOM	2535	С	PHE	1747	16.118	-11.227	3.522	1.00	23.18
ATOM	2536	0	PHE	1747	16.271	-11.873	4.548	1.00	24.04
ATOM	2537	N	LYS	1748	15.570	-11.745	2.432	1.00	24.13
ATOM	2539	CA	LYS	1748	15.137	-13.132	2.385	1.00	26.35
ATOM	2540	CB	LYS	1748	14.502	-13.424	1.024	1.00	27.52
ATOM	2541	CG	LYS	1748	14.034	-14.849	0.836	1.00	33.88
ATOM	2542	CD	LYS	1748	13.598	-15.062	-0.600	1.00	41.83
ATOM	2543	CE	LYS	1748	13.190	-16.506	-0.881	1.00	50.05
ATOM	2544	NZ	LYS	1748	12.084	-16.986	0.005	1.00	55.70
MOTA	2548	C	LYS	1748	16.359	-14.037	2.636	1.00	27.50
MOTA	2549	0	LYS	1748	16.303	-14.950	3.459	1.00	31.18
ATOM	2550	N	GLN	1749	17.467	-13.761	1.949	1.00	27.24
ATOM	2552	CA	GLN	1749	18.699	-14.529	2.122	1.00	27.03
ATOM	2553	CB	GLN	1749	19.797	-14.039	1.169	1.00	31.80
ATOM	2554	CG	GLN	1749	19.501	-14.196	-0.323	1.00	38.57
ATOM	2555	CD	GLN	1749	20.460	-13.385	-1.209	1.00	39.93
ATOM	2556	OE1	GLN	1749	20.025	-12.535	-1.974	1.00	39.90
ATOM	2557	NE2	GLN	1749	21.768	-13.620	-1.068	1.00	40.23
ATOM	2560	C	GLN	1749	19.205	-14.380	3.552	1.00	25.98
ATOM	2561	0	GLN	1749	19.533	-15.371	4.198	1.00	27.18
ATOM	2562	N	LEU	1750	19.293	-13.133	4.018	1.00	25.20
ATOM	2564	CA	LEU	1750	19.774	-12.823	5.369	1.00	25.74
ATOM	2565 2566	CB	LEU	1750	19.722	-11.317	5.631	1.00	20.99
ATOM ATOM	2566 2567	CG CD1	LEU LEU	1750	20.708	-10.468	4.831	1.00	20.90
ATOM	2568	CD1	LEU	1750 1750	20.302	-8.987 -10.643	4.822	1.00	19.88
ATOM	2569	CD2			22.071	-10.643	5.426	1.00	17.26
MION	4303	_	LEU	1750	18.985	-13.555	6.441	1.00	27.10



ATO	vi 2576								
ATO			LEU		19.553			1.00	27.89
ATON			VAL		17.672		6.265	1.00	29.40
ATOM			VAL		16.798	-	. – – •	1.00	26.80
ATOM			VAL		15.324			1.00	26.94
ATOM					14.429			1.00	
ATOM					14.941			1.00	24.10
ATOM		_	VAL		17.136	-15.745	7.228	1.00	27.80
ATOM			VAL		17.223	-16.359	8.285		26.77
ATOM			GLU	1752	17.408	-16.300	6.056	1.00	32.26
			GLU	1752	17.749	~17.717	5.966	1.00	35.72
ATOM ATOM			GLU	1752	17.721	-18.173	4.504	1.00	39.33
ATOM		CG	GLU		16.306	-18.078	3.911	1.00	49.41
		CD	GLU	1752	16.209	-18.421	2.429	1.00	55.88
ATOM		OE1	GLU	1752	15.141	-18.138	1.835	1.00	58.00
ATOM		OE2	GLU	1752	17.180	-18.978	1.863	1.00	61.03
ATOM		C	GLU	1752	19.093	-18.002	6.635	1.00	34.59
ATOM		0	GLU	1752	19.230	-18.975	7.393	1.00	33.95
ATOM		N	ASP	1753	20.057	-17.114	6.401	1.00	34.38
ATOM		CA	ASP	1753	21.393	-17.235	6.977	1.00	32.81
ATOM		CB	ASP	1753	22.338	-16.227	6.334	1.00	31.57
ATOM	2593	CG	ASP	1753	22.628	-16.556	4.888	1.00	33.68
ATOM	2594	OD1	ASP	1753	22.573	-17.755	4.536	1.00	35.14
ATOM	2595	OD2	ASP	1753	22.914	-15.624	4.104	1.00	34.44
ATOM	2596	C	ASP	1753	21.378	-17.058	8.489	1.00	32.04
ATOM	2597	O.	ASP	1753	21.997	-17.837	9.214	1.00	31.21
ATOM	2598	N	LEU	1754	20.648	-16.045	8.955	1.00	31.00
MOTA	2600	CA	LEU	1754	20.528	-15.754	10.382	1.00	29.46
ATOM	2601	CB	LEU	1754	19.822	-14.426	10.598	1.00	23.47
ATOM	2602	CG	LEU	1754	20.816	-13.309	10.318	1.00	23.58
ATOM	2603	CD1	LEU	1754	20.114	-11.963	10.128	1.00	20.46
ATOM	2604	CD2	LEU	1754	21.828	-13.282	11.462	1.00	19.18
ATOM	2605	C	LEU	1754	19.806	-16.866	11.110	1.00	31.84
ATOM	2606	0	LEU	1754	20.125	-17.178	12.254	1.00	30.78
ATOM	2607	N	ASP	1755	18.832	-17.471	10.445	1.00	34.03
ATOM	2609	CA	ASP	1755	18.116	-18.578	11.044	1.00	35.22
ATOM	2610	CB	ASP	1755	16.973	-19.027	10.148	1.00	38.40
ATOM ATOM	2611	CG	ASP	.1755	16.159	-20.119	10.779	1.00	41.85
ATOM	2612	OD1	ASP	1755	15.560	-19.866	11.841	1.00	47.90
	2613	OD2	ASP	1755	16.142	-21.241	10.238	1.00	46.67
ATOM	2614	C	ASP	1755	19.114	-19.724	11.222	1.00	36.79
ATOM	2615	C	ASP	1755	19.114	-20.411	12.250	1.00	38.33
ATOM	2616	N	ARG	1756	19.973	-19.920	10.226	1.00	34.81
MOTA	2618	CA	ARG	1756	20.982	-20.969	10.302	1.00	34.68
MOTA	2619	CB	ARG	1756	21.688	-21.100	8.959	1.00	34.78
ATOM	2620	CG	ARG	1756	22.746	-22.179	8.910	1.00	35.93
ATOM	2621	CD	ARG	1756	23.297	-22.306	7.511	1.00	41.60
ATOM	2622	NE	ARG	1756	23.786	-21.025	6.999	1.00	46.42
ATOM	2624	CZ	ARG	1756	24.889	-20.419	7.427	1.00	48.38
ATOM	2625	NH1	ARG	1756	25.637	-20.976	8.381	1.00	48.10
ATOM	2628	NH2	ARG	1756	25.236	-19.242	6.909	1.00	46.62
ATOM	2631	C	ARG	1756	22.002	-20.666	11.399	1.00	36.17
ATOM	2632	0	ARG	1756	22.372	-21.541	12.177	1.00	38.33
ATOM	2633	N	ILE	1757	22.433	-19.413	11.478	1.00	37.00
ATOM	2635	CA	ILE	1757	23.416	-18.998	12.468	1.00	
									35.60



ATOM	2636	CB	ILE	1757	23.964	-17.588	12.141	1.00	35.54
MOTA	2637	CG2	ILE	1757	24.921	-17.131	13.217	1.00	32.41
ATOM	2638	CG1	ILE	1757	24.693	-17.612	10.794	1.00	33.77
MOTA	2639	CD1	ILE	1757	25.097	-16.253	10.287	1.00	33.49
MOTA	2640	C	ILE	1757	22.866	-19.048	13.891	1.00	37.28
ATOM	2641	0	ILE	1757	23.531	-19.556	14.779	1.00	38.42
ATOM	2642	N	VAL	1758	21.634	-18.585	14.088	1.00	39.19
ATOM	2644	CA	VAL	1758	21.016	-18.584	15.421	1.00	39.84
MOTA	2645	CB	VAL	1758	19.560	-18.017	15.403	1.00	37.62
ATOM	2646	CG1	VAL	1758	18.918	-18.144	16.773	1.00	38.30
MOTA	2647	CG2	VAL	1758	19.560	-16.560	15.009	1.00	39.62
ATOM	2648	С	VAL	1758	20.983	-19.997	15.988	1.00	41.98
ATOM	2649	0	VAL	1758	21.380	-20.229	17.128	1.00	43.36
ATOM	2650	N	ALA	1759	20.501	-20.932	15.182	1.00	43.31
ATOM	2652	CA	. ALA	1759	20.418	-22.325	15.589	1.00	44.00
ATOM	2653	CB	ALA	1759	19.836	-23.150	14.459	1.00	44.52
ATOM	2654	C	ALA	1759	21.784	-22.867	15.976	1.00	45.98
ATOM	2655	0	ALA	1759	21.894	-23.725	16.841	1.00	48.78
ATOM	2656	И	LEU	1760	22.823	-22.375	15.319	1.00	48.93
ATOM	2658	CA	LEU	1760	24.175	-22.831	15.592	1.00	51.47
ATOM	2659	CB	LEU	1760	24.954	-22.900	14.280	1.00	53.63
ATOM	2660	CG	LEU	1760	24.284	-23.864	13.295	1.00	57.84
ATOM	2661	CD1	LEU	1760	24.993	-23.847	11.948	1.00	61.83
ATOM	2662	CD2	LEU	1760	24.260	-25.277	13.886	1.00	58.57
ATOM ATOM	2663	С 0	LEU	1760	24.911	-21.965	16.607	1.00	53.60
ATOM	2664	JN	LEU	1760	26.078	-22.214	16.919	1.00	54.00
ATOM	2665 2667	CA	THR	1761	24.222	-20.963	17.141	1.00	55.77
ATOM	2668	CB	THR THR	1761	24.820	-20.060	18.111	1.00	56.64
ATOM	2669	OG1	THR	1761 1761	24.250	-18.627	17.979	1.00	55.76
ATOM	2671	CG2	THR	1761	24.444 24.962	-18.154	16.644	1.00	56.20
ATOM	2672	C	THR	1761	24.636	-17.680 -20.548	18.917 19.539	1.00	55.25
ATOM	2673	0	THR	1761	23.566	-21.021	19.919	1.00	58.16 56.85
MOTA	2674	И	SER	1762	25.706	-20.436	20.318	1.00	61.74
ATOM	2676	CA	SER	1762	25.706	-20.833	21.717	1.00	64.50
ATOM	2677	CB	SER	1762	27.155	-20.979	22.205	1.00	68.82
ATOM	2678	OG	SER	1762	27.232	-21.544	23.508	1.00	73.15
ATOM	2680	С	SER	1762	24.965	-19.775	22.547	1.00	63.87
ATOM	2681	0	SER	1762	25.080	-18.563	22.296	1.00	63.22
ATOM	3420	PA	PCP	400	62.748	10.301	7.817	1.00	90.90
MOTA	3421	01A	PCP	400	62.509	10.036	9.280	1.00	92.35
ATOM	3422	02A	PCP	400	61.832	11.180	7.038	1.00	90.49
MOTA	3423	05*	PCP	400	62.744	8.904	7.142	1.00	83.57
ATOM	3424	PB	PCP	400	65.226	11.946	8.294	1.00	101.51
MOTA	3425	OlB	PCP	400	65.246	13.015	7.264	1.00	102.85
ATOM	3426	02B	PCP	400	66.527	11.458	8.830	1.00	99.88
ATOM	3427	AEO	PCP	400	64.334	10.725	7.584	1.00	96.64
ATOM	3428	C3B	PCP	400	64.345	12.502	9.635	1.00	102.94
ATOM	3429	C5*	PCP	400	62.337	8.684	5.839	1.00	71.21
ATOM	3430	C4*	PCP	400	62.479	7.204	5.587	1.00	64.48
MOTA	3431	04 *	PCP	400	63.713	6.745	6.169	1.00	60.91
MOTA	3432	C1*	PCP	400	63.394	5.459	6.680	1.00	54.96
MOTA	3433	N9	PCP	400	64.326	5.101	7.712	1.00	47.26
ATOM	3434	C4	PCP	400	65.017	3.903	7.840	1.00	46.24

ATO		5 N3	PCI	400	64.926	2.770	7.062	1.00	41.02
ATO		C2	PCI	400	65.802	1.878			
ATO	4 3437	7 N1	PCI	400	66.674	1.917			
ATO		C6	PCF	400	66.735	3.028			
ATON			PCF	400	67.573	3.134			
ATOM		C5	PCF	400	65.862	4.091			
ATOM	1 3443	N7	PCP	400	65.674	5.361			44.12
ATOM	3444	C8	PCP	400	64.761	5.894	- · - · <del>-</del>		45.15
ATOM	3445	C2*	PCP	400	61.986	5.500		1.00	44.83
ATOM	3446	02*	PCP	400	61.454	4.153	7.211	1.00	57.63
ATOM	3448	C3 *	PCP		61.328	6.402		1.00	56.45
ATOM		03*	PCP	400	60.689	5.644	6.245	1.00	61.31
ATOM	3451	PA	PCP		9.366	9.801	5.206	1.00	64.65
ATOM	3452	Ola			9.463	8.736	17.743	0.50	74.43
ATOM	3453	O2A	PCP		10.330	10.926	16.709	0.50	75.37
ATOM	3454	05*	PCP		9.427	9.108	17.699	0.50	75.86
ATOM	3455	PB	PCP	401	6.878	10.679	19.186	0.50	67.44
ATOM	3456	OlB	PCP	401	6.223	11.982	16.547	0.50	82.27
ATOM	3457	02B	PCP	401	6.020		16.778	0.50	82.91
ATOM	3458	03A	PCP	401	7.868	9.486	16.408	0.50	82.70
ATOM	3459	C3B	PCP	401	7.790	10.423 10.845	17.814	0.50	78.30
MOTA	3460	C5*	PCP	401	10.184		15.159	0.50	82.50
ATOM	3461	C4*	PCP	401	10.228	9.593	20.275	0.50	54.44
ATOM	3462	04 *	PCP	401	9.032	8.637	21.442	0.50	45.36
ATOM	3463	C1*	PCP	401	9.397	7.855	21.412	0.50	39.40
ATOM	3464	N9	PCP	401	8.386	6.509 5.627	21.641	0.50	35.00
ATOM	3465	C4	PCP	401	7.790		21.044	0.50	27.91
ATOM	3466	N3	PCP	401	7.982	4.469 3.849	21.564	0.50	23.36
ATOM	3467	C2	PCP	401	7.239	2.768	22.732	0.50	22.33
ATOM	3468	N1	PCP	401	6.382	2.251	22.838	0.50	20.26
ATOM	3469	C6	PCP	401	6.202	2.877	22.003	0.50	17.29
ATOM	3470	N6	PCP	401	5.327	2.415	20.856	0.50	19.35
ATOM	3473	C5	PCP	401	6.932	4.038	19.975	0.50	16.87
MOTA	3474	N7	PCP	401	6.983	4.880	20.603 19.507	0.50	21.72
MOTA	3475	C8	PCP	401	7.847	5.786	19.507	0.50	24.59
ATOM	3476	C2*	PCP	401	10.762	6.409		0.50	24.26
ATOM	3477	02*	PCP	401	11.609	5.326	20.931 21.412	0.50	39.01
ATOM	3479	C3*	PCP	401	11.396	7.674	21.412	0.50	43.88
MOTA	3480	03*	PCP	401	11.918	7.515	22.681	0.50	42.14
MOTA	3482	N	SER	461	78.844	26.057		0.50	44.21
MOTA	3484	CA	SER	461	79.399	24.884	14.057	1.00	43.87
ATOM	3485	CB	SER	461	78.488	23.655	13.385	1.00	43.50
ATOM	3486	С	SER	461	79.572	25.181	13.616	1.00	39.99
MOTA	3487	0	SER	461	79.473	24.292	11.888	1.00	42.14
MOTA	3488	N	GLU	462	79.883	26.441	11.038	1.00	40.29
ATOM	3490	CA	GLU	462	80.061	26.951	11.594	1.00	43.19
ATOM	3491	СВ	GLU	462	80.303	28.446	10.233	1.00	42.77
ATOM	3492	CG	GLU	462	79.209		10.250		47.75
ATOM	3493	CD	GLU	462	79.647	29.301	10.860		60.57
ATOM	3494	OE1	GLU	462	80.866	30.752	11.061		67.56
ATOM	3495	OE2	GLU	462	78.764	31.016	10.994		67.47
ATOM	3496	C	GLU	462	81.207	31.611			72.32
ATOM	3497	0	GLU	462	81.207 81.051	26.357	9.457		39.55
ATOM	3498	N	TYR	463	81.051 82.375	26.032			38.74
	_		• `	103	04.3/5	26.299	10.091	1.00	36.47

ATOM	3500	CA	TYR	463	83.567	25.806	9.420	1.00	34.19
ATOM	3501	CB	TYR	463	84.702	26.828	9.505	1.00	35.55
ATOM	3502	CG	TYR	463	84.393	28.059	8.675	1.00	42.11
MOTA	3503	CD1	TYR	463	84.004	29.264	9.283	1.00	43.15
MOTA	3504	CE1	TYR	463	83.619	30.361	8.513	1.00	42.40
ATOM	3505	CD2	TYR	463	84.395	27.990	7.280	1.00	39.78
MOTA	3506	CE2	TYR	463	84.012	29.078	6.509	1.00	39.04
ATOM	3507	CZ	TYR	463	83.625	30.256	7.129	1.00	39.86
ATOM	3508	OH	TYR	463	83.260	31.330	6.366	1.00	42.58
ATOM	3510	C	TYR	463	84.055	24.434	9.800	1.00	33.28
ATOM	3511	0	TYR	463	84.739	23.781	9.005	1.00	33.47
ATOM	3512	N	GLU	464	83.695	23.976	10.993	1.00	34.42
ATOM	3514	CA	GLU	464	84.117	22.660	11.444	1.00	36.38
ATOM	3515	CB	GLU	464	85.618	22.663	11.750	1.00	40.90
MOTA	3516	CG	GLU	464	86.041	23.755	12.729	1.00	46.29
MOTA	3517	CD	GLU	464	87.548	23.810	12.943	.1.00	51.33
MOTA	3518	OE1	GLU	464	87.970	24.247	14.038	1.00	54.49
ATOM	3519	OE2	GLU	464	88.312	23.430	12.025	1.00	53.18
MOTA	3520	С	GLU	464	83.374	22.224	12.678	1.00	35.64
MOTA	3521	O	GLU	464	83.111	23.052	13.555	1.00	37.40
ATOM	3522	N	LEU	465	82.962	20.955	12.711	1.00	34.21
ATOM	3524	CA	LEU	465	82.267	20.429	13.887	1.00	34.92
ATOM	3525	CB	LEU	465	81.285	19.300	13.542	1.00	31.30
ATOM	3526	CG	LEU	465	80.272	19.381	12.405	1.00	32.22
ATOM	3527	CD1	LEU	465	79.152	18.407	12.720	1.00	21.95
ATOM	3528	CD2	LEU	465	79.738	20.802	12.212	1.00	29.75
ATOM	3529	C	LEU	465	83.326	19.855	14.814	1.00	36.17
ATOM	3530	0	LEU	465	84.473	19.621	14.400	1.00	35.80
ATOM	3531 3532	N	PRO	466	82.970	19.629	16.083	1.00	36.20
ATOM	3532	CD CA	PRO PRO	466 466	81.722	20.019	16.758	1.00	38.17
ATOM	3534	CB	PRO	466	83.925	19.072	17.037	1.00	36.06
ATOM	3535	CG	PRO	466	83.132 82.185	19.035 20.194	18.333	1.00	35.57
ATOM	3536	C	PRO	466	84.294	17.666	18.171 16.605	1.00	38.67
ATOM	3537	ō	PRO	466	83.498	16.959	15.979	1.00	37.06 34.50
ATOM	3538	N	GLU	467	85.504	17.258	16.936	1.00	39.97
ATOM	3540	CA	GLU	467	85.951	15.932	16.587	1.00	44.69
ATOM	3541	СВ	GLU	467	87.412	15.985	16.151	1.00	50.43
ATOM	3542	CG	GLU	467	87.902	14.695	15.518	1.00	60.27
MOTA	3543	CD	GLU	467	89.321	14.796	14.986	1:00	65.75
MOTA	3544	OE1	GLU	467	90.024	15.804	15.269	1.00	64.40
ATOM	3545	OE2	GLU	467	89.726	13.850	14.275	1.00	71.13
ATOM	3546	C	GLU	467	85.775	15.002	17.783	1.00	43.30
ATOM	3547	0	GLU	467	85.888	15.428	18.936	1.00	43.26
ATOM	3548	N	ASP	468	85.433	13.750	17.504	1.00	43.09
MOTA	3550	CA	ASP	468	85.254	12.739	18.545	1.00	44.15
MOTA	3551	CB	ASP	468	83.785	12.614	18.979	1.00	44.54
MOTA	3552	CG	ASP	468	83.574	11.562	20.072	1.00	41.84
ATOM	3553	OD1	ASP	468	82.405	11.244	20.368	1.00	39.81
ATOM	3554	OD2	ASP	468	84.570	11.057	20.636	1.00	42.92
MOTA	3555	С	ASP	468	85.746	11.422	17.970	1.00	44.66
ATOM	3556	0	ASP	468	84.982	10.663	17.368	1.00	44.56
ATOM	3557	N	PRO	469	87.034	11.126	18.176	1.00	44.56
ATOM	3558	CD	PRO	469	87.953	11.959	18.971	1.00	45.43



ATOM			PRO	469	87.707	9.916	17.707	1.00	43.90
ATOM		CB	PRO	469	89.024	9.959	18.476	1.00	
ATOM			PRO	469	89.300	11.438	18.547	1.00	
ATOM			PRO	469	86.934	8.627	17.971	1.00	42.60
MOTA		0	PRO	469	86.935	7.730	17.139	1.00	41.35
MOTA	3564	N	ARG	470	86.229	8.569	19.096	1.00	43.25
MOTA	3566	CA	ARG	470	85.460	7.380	19.470	1.00	44.81
ATOM	3567	CB	ARG	470	84.722	7.612	20.789	1.00	48.36
ATOM	3568	CG	ARG	470	85.579	8.201	21.889	1.00	53.41
ATOM	3569	CD	ARG	470	84.764	8.458	23.138	1.00	55.42
ATOM	3570	NE	ARG	470	83.581	9.261	22.861	1.00	58.57
ATOM	3572	CZ	ARG	470	82.748	9.712	23.791	1.00	
ATOM	3573	NH1	ARG	470	82.972	9.445	25.077	1.00	62.24
ATOM	3576	NH2	ARG	470	81.670	10.398	23.436		64.57
ATOM	3579	C	ARG	470	84.439	6.924	18.437	1.00	63.66
ATOM	3580	0	ARG	470	84.166	5.735	18.313	1.00	43.69
ATOM	3581	N	TRP	471	83.879	7.866	17.693	1.00	45.68
ATOM	3583	CA	TRP	471	82.851	7.534	16.720	1.00	42.41
MOTA	3584	CB	TRP	471	81.577	8.268	17.095	1.00	38.92
ATOM	3585	CG	TRP	471	80.967	7.741	18.335	1.00	35.80
ATOM	3586	CD2	TRP	471	80.158	6.569	18.443	1.00	37.13
ATOM	3587	CE2	TRP	471	79.723	6.483		1.00	37.26
ATOM	3588	CE3	TRP	471	79.748	5.582	19.785	1.00	38.20
ATOM	3589	CD1	TRP	471	81.010	8.300	17.530	1.00	35.59
ATOM	3590	NEl	TRP	471	80.260	7.553	19.584	1.00	36.42
ATOM	3592	CZ2	TRP	471	78.896	5.454	20.462	1.00	35.89
ATOM	3593	CZ3	TRP	471	78.934	4.561	20.239 17.978	1.00	36.18
ATOM	3594	CH2	TRP	471	78.514	4.505	19.321	1.00	32.81
ATOM	3595	C:	TRP	471	83.175	7.845	15.277	1.00	34.82
ATOM	3596	0	TRP	471	82.478	7.391	14.362	1.00	39.77
ATOM	3597	N	GLU	472	84.224	8.628	15.075	1.00	39.56
ATOM	3599	CA	GLU	472	84.605	9.043	13.739	1.00	39.37
ATOM	3600	CB	GLU	472	85.794	9.994	13.812	1.00	38.42
ATOM	3601	CG	GLU	472	85.958	10.849	12.582	1.00	37.11
MOTA	3602	CD	GLU	472	84.772	11.757	12.338	1.00	34.11
ATOM	3603	OE1	GLU	472	84.260	12.348	13.317	1.00	34.03
ATOM	3604	OE2	GLU	472	84.367	11.885	11.163	1.00	31.87
MOTA	3605	С	GLU	472	84.910	7.901	12.791	1.00	32.11
MOTA	3606	0	GLU	472	85.656	6.975	13.128	1.00	39.78 41.64
ATOM	3607	N	LEU	473	84.303	7.958	11.610	1.00	37.71
ATOM	3609	CA	LEU	473	84.538	6.957	10.590	1.00	
ATOM	3610	CB	LEU	473	83.258	6.196	10.265	1.00	36.94
MOTA	3611	CG	LEU	473	83.438	5.065	9.236		35.38
ATOM	3612	CD1	LEU	473	84.070	3.845	9.903	1.00	37.67
ATOM	3613	CD2	LEU	473	82.106	4.687		1.00	37.28
ATOM	3614	С	LEU	473	85.035	7.664	8.598	1.00	37.87
ATOM	3615	0	LEU	473	84.484	8.697	9.330	1.00	39.31
MOTA	3616	N	PRO	474	86.140	7.164	8.938	1.00	40.55
MOTA	3617	CD	PRO	474	87.052	6.170	8.732	1.00	39.20
ATOM	3618	CA	PRO	474	86.735	7.716	9.327	1.00	37.83
ATOM	3619	CB	PRO	474	87.914		7.513	1.00	38.53
ATOM	3620	CG	PRO	474	88.355	6.777	7.282	1.00	37.16
ATOM	3621	C	PRO	474		6.488	8.644	1.00	34.42
ATOM	3622	0	PRO	474	85.733 85.220	7.607	6.370	1.00	40.25
		~	11.0	z / Z	05.220	6.523	6.098	1.00	40.70

ATOM	3623	N	ARG	475	85.492	8.723	5.685	1.00	41.09
ATOM	3625	CA	ARG	475	84.534	8.746	4.590	1.00	42.26
MOTA	3626	CB	ARG	475	84.487	10.132	3.948	1.00	39.19
MOTA	3627	CG	ARG	475	83.957	11.199	4.876	1.00	35.19
ATOM	3628	CD	ARG	475	84.074	12.593	4.301	1.00	30.76
MOTA	3629	NE	ARG	475	83.796	13.567	5.345	1.00	22.86
MOTA	3631	CZ	ARG	475	82.581	13.898	5.748	1.00	21.99
MOTA	3632	NH1	ARG	475	81.529	13.350	5.165	1.00	23.39
ATOM	3635	NH2	ARG	475	82.412	14.662	6.813	1.00	22.55
ATOM	3638	C	ARG	475	84.838	7.692	3.538	1.00	45.38
ATOM	3639	0	ARG	475	83.927	7.182	2.892	1.00	47.15
ATOM	3640	N	ASP	476	86.106	7.319	3.390	1.00	47.13
ATOM	3642	CA	ASP	476	86.461	6.325	2.387	1.00	51.33
ATOM	3643	CB	ASP	476	87.973	6.294	2.134	1.00	55.23
ATOM	3644	CG	ASP	476	88.768	5.841	3.340	1.00	61.16
ATOM	3645	OD1	ASP	476	88.863	4.617	3.573	1.00	65.55
ATOM	3646	OD2	ASP	476	89.331	6.713	4.036	1.00	65.78
MOTA	3647	C	ASP	476	85.932 .	4.940	2.746	1.00	52.35
MOTA	3648	С	ASP	476	85.815	4.063	1.885	1.00	55.49
ATOM	3649	N	ARG	477	85.609 -	4.752	4.021	1.00	50.77
ATOM	3651	CA	ARG	477	85.080	3.482	4.508	1.00	48.65
ATOM	3652	CB	ARG	477	85.612	3.208	5.908	1.00	50.02
ATOM	3653	CG	ARG	477	87.067	2.799	5.881	1.00	55.33
ATOM	3654	CD	ARG	477	87.760	3.030	7.201	1.00	60.38
MOTA	3655	NE	ARG	477	87.238	2.207	8.285	1.00	64.36
ATOM	3657	CZ	ARG	477	87.748	2.203	9.513	1.00	69.16
ATOM	3658	NH1	ARG	477	88.794	2.968	9.814	1.00	70.73
ATOM	3661	NH2	ARG	477	87.190	1.459	10.159	1.00	71.59
ATOM	3664	С	ARG	477	83.546	3.414	4.484	1.00	46.25
ATOM	3665	0	ARG	477	82.957	2.481	5.013	1.00	46.36
ATOM	3666	N	LEU	478	82.913	4.372	3.815	1.00	42.23
MOTA	3668	CA	LEU	478	81.464	4.418	3.743	1.00	38.89
ATOM	3669	CB	LEU	478	80.938	5.537	4.657	1.00	37.17
ATOM	3670	CG	LEU	478	79.418	5.733	4.678	1.00	34.13
ATOM	3671	CD1	LEU	478	78.777	4.723	5.609	1.00	32.24
MOTA MOTA	3672	CD2	LEU	478	79.074	7.133	5.101	1.00	33.15
ATOM	3673 3674	С О	LEU	478	81.059	4.697	2.303	1.00	38.34
ATOM	3675	N	LEU VAL	478 479	81.515	5.671	1.711	1.00	40.88
ATOM	3677	CA	LAV	479	80.208 79.763	3.850	1.738	1.00	37.34
ATOM	3678	CB	VAL	479	80.105	4.042	0.364	1.00	37.61
ATOM	3679	CG1	VAL	479	79.647	2.829	-0.563	1.00	36.57
ATOM	3680	CG2	VAL	479	81.608	3.105	-1.994	1.00	31.59
ATOM	3681	C	VAL	479	78.267	2.567	-0.561	1.00	36.11
ATOM	3682	0	VAL	479	77.484	4.277	0.375	1.00	39.24
ATOM	3683	N	LEU	480	77.894	3.358 5.528	0.619	1.00	39.16
ATOM	3685	CA	LEU	480	76.505	5.960	0.142	1.00	41.32
ATOM	3686	СВ	LEU	480	76.446	7.480	0.123 -0.008		41.60,
ATOM	3687	CG	LEU	480	77.129	8.257		1.00	41.31
ATOM	3688	CD1	LEU	480	76.985	9.737	1.118 0.856	1.00	39.82
ATOM	3689	CD2	LEU	480	76.563	7.887	2.458	1.00	37.96
ATOM	3690	C	LEU	480	75.733	5.312	-1.015	1.00	37.70
ATOM	3691	0	LEU	480	76.235	5.224	-2.131	1.00	41.85
ATOM	3692	N	GLY	481	74.501	4.897	-0.727	1.00	45.02 40.86
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MOTA 3694 GLY 481 73.673 4.247 CA -1.727 1.00 40.21 **ATOM** 3695 C, . GLY 481 72.270 4.806 -1.873 1.00 39.78 MOTA 3696 0 GLY 481 72.058 6.015 -1.810 1.00 41.68 ATOM 3697 482 N LYS 71.306 3.914 -2.063 1.00 39.98 69.910 MOTA 3699 CA LYS 482 4.297 -2.249 1.00 42.13 MOTA 3700 CB LYS 482 69.061 3.056 -2.566 1.00 42.73 MOTA 3701 C LYS 482 69.284 5.050 -1.084 1.00 43.13 ATOM 3702 0 LYS 482 69.373 4.625 0.060 1.00 44.49 ATOM 3703 PRO N 483 68.676 6.204 -1.358 1.00 43.22 MOTA 3704 CD PRO 483 68.708 6.969 -2.613 1.00 44.40 MOTA 3705 CA PRO 483 68.044 6.973 -0.290 1.00 45.44 ATOM 3706 CB PRO 483 67.701 8.295 -0.980 1.00 45.01 ATOM 3707 PRO CG 483 67.573 7.923 -2.414 1.00 43.95 ATOM 3708 PRO C 483 66.801 6.261 0.232 47.67 1.00 **ATOM** 3709 0 PRO 483 66.012 5.725 -0.547 1.00 46.76 MOTA 3710 N LEU 484 66.650 6.242 1.552 1.00 49.68 MOTA 3712 LEU CA 484 65.514 5.598 2.196 1.00 54.51 MOTA 3713 CB LEU 484 65.935 5.026 3.555 1.00 52.70 MOTA 3714 CG LEU 484 67.132 4.066 3.530 1.00 51.83 **ATOM** 3715 CD1 LEU 484 67.620 3.766 4.933 1.00 50.19 **ATOM** 3716 CD2 LEU 484 66.755 2.788 2.825 1.00 52.22 ATOM 3717 LEU 484 C 64.317 6.554 2.357 1.00 58.82 ATOM 3718 LEU 484 O 63.158 6.138 2.244 1.00 60.07 MOTA 3719 GLY N 485 64.599 7.831 2.609 1.00 61.91 ATOM 3721 GLY 485 CA 63.538 8.810 2.778 1.00 65.89 MOTA 3722 C GLY 485 64.057 10.167 3.227 1..00 69.46 MOTA 3723 O GLY 485 65.230 10.301 1.00 3.597 70.65 ATOM 3724 GLU N 486 63.178 : 11.165 · 3.241 1.00 70.72 MOTA 3726 CA GLU 486 63.563 12.521 1.00 3.624 71.32 MOTA 3727 CB GLU 486 64.015 13.298 2.389 1.00 73.69 ATOM 3728 C GLU 486 62.435 13.269 4.312 1.00 70.93 ATOM 3729 0 GLU 486 61.281 12.846 4.275 1.00 71.58 ATOM 3730 N GLY 487 62.781 14.404 4.909 1.00 70.10 MOTA 3732 CA GLY 487 61.798 15.211 5.603 1.00 68.11 MOTA 3733 C GLY 487 62.218 16.669 5.598 1.00 67.97 MOTA 3734 0 GLY 487 62.938 17.109 4.696 1.00 67.68 MOTA 37.35 N ALA 488 61.780 17.409 6.615 1 00 67.26 6.737 ATOM 3737 CA ALA 488 62.106 18.826 1.00 66.90 ATOM 3738 CB ALA 488 7.909 1.00 61.362 19.428 68.72 ATOM 3739 C ALA 488 63.607 19.004 6.921 1.00 67.08 MOTA 3740 488 0 ALA 64.124 18.867 8.037 1.00 65.97 MOTA 3741 N PHE 489 64.297 19.248 5.806 1.00 66.76 **ATOM** 3743 CA PHE 489 65.754 19.439 5.773 1.00 65.91 ATOM 3744 CB PHE 489 20.794 1.00 66.134 6.379 66.45 MOTA 3745 PHE 489 66.563 18.288 6.414 1.00 С 63.92 **ATOM** 3746 0 PHE 489 67.622 18.503 7.031 1.00 63.16 MOTA 3747 N GLY 490 66.067 17.069 6.209 1.00 59.03 ATOM 3749 CA GLY 490 66.710 15.878 6.720 1.00 51.12 **ATOM** 3750 C GLY 490 14.823 1.00 66.619 5.638 48.59 MOTA GLY 3751 0 490 65.608 14.736 4.938 1.00 45.25 MOTA 3752 GLN 491 67.659 14.003 5.525 N 1.00 48.77 67.732 MOTA 3754 GLN CA 491 12.951 4.519 1.00 47.40 MOTA 3755 CB GLN 491 68.529 13.474 3.319 1.00 49.92 MOTA 3756 CG GLN 491 68.653 12.514 2.155 1.00 56.31

ATOM	3757	CD	GLN	491	69.604	13.020	1.088	1.00	58.79
ATOM	3758	OE1	GLN	491	70.043	14.171	1.130	1.00	59.63
MOTA	3759	NE2	GLN	491	69.929	12.161	0.122	1.00	59.05
ATOM	3762	C	GLN	491	68.407	11.693	5.086	1.00	44.46
ATOM	3763	0	GLN	491	69.396	11.782	5.806	1.00	44.15
ATOM	3764	N	VAL	492	67.867	10.527	4.752	1.00	42.55
MOTA	3766	CA	VAL	492	68.416	9.247	5.205	1.00	39.22
ATOM	3767	CB	VAL	492	67.375	8.458	6.042	1.00	39.40
MOTA	3768	CGl	VAL	492	67.947	7.127	6.524	1.00	40.17
MOTA	3769	CG2	VAL	492	66.922	9.267	7.210	1.00	36.12
MOTA	3770	С	VAL	492	68.746	8.396	3.975	1.00	37.57
MOTA	3771	0	VAL	492	67.888	8.178	3.115	1.00	35.70
MOTA	3772	N	VAL	493	69.990	7.961	3.845	1.00	36.27
ATOM	3774	CA	VAL	493	70.333	7.127	2.711	1.00	37.61
MOTA	3775	CB	VAL	493	71.237	7.863	1.643	1.00	37.45
MOTA	3776	CG1	VAL	493	70.836	9.319	1.524	1.00	38.29
ATOM	3777	CG2	VAL	493	72.717	7.713	1.943	1.00	36.53
ATOM	3778	С	VAL	493	70.952	5.806	3.156	1.00	37.54
ATOM	3779	0	VAL	493	71.542	5.711	4.233	1.00	37.32
ATOM	3780	N	LEU	494	70.691	4.763	2.380	1.00	37.67
ATOM	3782	CA	LEU	494	71.236	3.450	2.656	1.00	38.41
ATOM	3783	CB	LEU	494	70.482	2.387	1.851	1.00	39.16
MOTA	3784	CG	LEU	494	70.834	0.908	2.021	1.00	36.43
ATOM	3785	CD1	LEU	494	70.809	0.508	3.479	1.00	34.69
ATOM	3786	CD2	LEU	494	69.840	0.086	1.229	1.00	37.48
ATOM	3787	С	LEU	494	72.683	3.541	2.202	1.00	39.30
ATOM	3788	0	LEU	494	72.976	4.201	1.207	1.00	39.21
ATOM	3789	N	ALA	495	73.584	2.922	2.954	1.00	40.08
ATOM	3791	CA	ALA	495	74.996	2.954	2.619	1.00	41.70
ATOM	3792	CB	ALA	495	75.654	4.162	3.283	1.00	41.63
ATOM	3793	C	ALA	495	75.670	1.669	3.080	1.00	43.92
MOTA	3794	0	ALA	495	75.033	0.818	3.711	1.00	45.20
MOTA	3795	N	GLU	496	76.946	1.515	2.731	1.00	44.21
MOTA	3797	CA	GLU	496	77.712	0.347	3.137	1.00	43.44
MOTA.	3798	CB	GLU	496		-0.538	1.943	1.00	45.87
ATOM	3799	CG	GLU	496	76.816	-1.142	1.301	1.00	53.11
ATOM	3800	CD	GLU	496	77.145	-2.262	0.339	1.00	56.68
MOTA	3801	OE1	GLU	496	76.473	-3.316	0.410	1.00	61.87
MOTA	3802	OE2	GLU	496	78.068	-2.091	-0.482	1.00	58.18
MOTA	3803	С	GLU	496	78.973	0.773	3.860	1.00	40.97
MOTA	3804	0	GLU	496	79.835	1.437	3.302	1.00	40.91
MOTA	3805	N	ALA	497	79.036	0.439	5.136	1.00	42.07
MOTA	3807	CA	ALA	497	80.173	0.786	5.959	1.00	43.69
ATOM	3808	CB	ALA	497	79.709	1.104	7.366	1.00	40.90
ATOM	3809	С	ALA	497	81.160	-0.372	5.962	1.00	46.16
MOTA	3810	0	ALA	497	80.764	-1.525	5.814	1.00	46.90
MOTA	3811	N	ILE	498	82.446	-0.059	6.090	1.00	48.78
MOTA	3813	CA	ILE	498	83.494	-1.068	6.114	1.00	49.59
ATOM	3814	СВ	ILE	498	84.395	-0.993	4.858	1.00	49.46
MOTA	3815	CG2	ILE	498	85.524	-2.006	4.954	1.00	51.16
ATOM	3816	CG1	ILE	498	83.577	-1.244	3.591	1.00	48.96
ATOM	3817	CD1	ILE	498	82.924	0.009	2.998	1.00	52.50
ATOM	3818	C	ILE	498	84.352	-0.877	7.355	1.00	51.33
ATOM	3819	0	ILE	498	84.818	0.230	7.641	1.00	50.42
							,	1.50	JU. 42

ATOM	3820	N	GLY	499	84.506	-1.952	8.119	1.00	53.87
MOTA	3822	CA	GLY	499	85.314	-1.909	9.324	1.00	58.16
ATOM	3823	C	GLY	499	84.759	-1.094	10.483	1.00	62.44
MOTA	3824	0	GLY	499	85.510	-0.400	11.175	1.00	65.17
ATOM	3825	N	LEU	500	83.454	-1.187	10.720	1.00	62.92
MOTA	3827	CA	LEU	500	82.839	-0.453	11.822	1.00	61.93
MOTA	3828	CB	LEU	500	81.339	-0.752	11.888	1.00	58.77
ATOM	3829	CG	LEU	500	80.501	-0.207	10.736	1.00	56.68
ATOM	3830	CD1	LEU	500	79.047	-0.547	10.964	1.00	55.05
ATOM	3831	CD2	LEU	<b>50</b> 0	80.682	1.298	10.635	1.00	56.30
ATOM	3832	C	LEU	500	83.501	-0.820	13.149	1.00	63.28
MOTA	3833	0	LEU	500	83.623	-2.002	13.487	1.00	64.91
MOTA	3834	N	PRO	505	87.387	-6.451	10.091	1.00	82.92
ATOM	3835	CD	PRO	505	88.522	-6.966	10.874	1.00	83.74
ATOM	3836	CA	PRO	505	87.618	-5.052	9.705	1.00	80.73
ATOM	3837	CB	PRO	505	89.027	-4.770	10.247	1.00	81.95
ATOM	3838	CG	PRO	505	89.655	-6.133	10.342	1.00	83.54
ATOM	3839	С	PRO	505	87.514	-4.794	8.205	1.00	77.60
ATOM	3640	0	PRO	505	87.445	-3.651	7.761	1.00	77.24
ATOM	3841	N	ASN	506	87.488	-5.863	7.424	1.00	75.24
ATOM	3843	CA	ASN	506	87.380	-5.727	5.981	1.00	72.92
ATOM	3844	CB	ASN	506	88.435	-6.589	5.283	1.00	73.87
ATOM	3845	C	ASN	506	85.978	-6.122	5.529	1.00	70.43
MOTA	3846	0	ASN	506	85.719	-6.281	4.340	1.00	70.01
ATOM	3847	N	ARG	507	85.075	-6.273	6.491	1.00	68.31
ATOM	3849	CA	ARG	507	83.697	-6.647	6.200	1.90	65.59
ATOM	3850	CB	ARG	507	83.112	-7.429	7.378	1.00	66.34
ATOM	3851	C	ARG	507	82.846	-5.413	5.941	1.00	62.97
ATOM	3852	0	ARG	507	83.191	-4.313	6.375	1.00	63.16
ATOM	3853	N	VAL	508	81.740	-5.599	5.231	1.00	60.02
ATOM	3855	CA	VAL	508	80.840	-4.495	4.947	1.00	58.59
ATOM ATOM	3856	CB	VAL	508	80.532	-4.357	3.439	1.00	58.40
ATOM	3857 3858	CG1 CG2	VAL VAL	508 508	81.813	-4.196	2.658	1.00	61.14
ATOM	3859	C	VAL	508	79.751	-5.553	2.938	1.00	61.01
ATOM	3860	0	VAL		79.537	-4.682	5.707	1.00	57.24
ATOM	3861	N	THR	508 509	79.031	-5.803	5.836	1.00	58.42
ATOM	3863	CA	THR	509	79.020	-3.579	6.237	1.00	54.22
ATOM	3864	CB	THR	509	77.769 77.971	-3.572	6.973	1.00	48.99
ATOM	3865	OG1	THR	509	78.932	-3.100	8.428	1.00	49.59
ATOM	3867	CG2	THR	509	76.932	-3.935 -3.166	9.082	1.00	51.71
ATOM	3868	C	THR	509	76.837	-3.166 -2.606	9.198	1.00	50.69
ATOM	3869	0	THR	509	77.231	-1.503	6.253	1.00	46.51
ATOM	3870	N	LYS	510	75.628	-3.059	5.886 5.966	1.00	44.91
ATOM	3872	CA	LYS	510	74.658	-2.208		1.00	45.65
ATOM	3873	CB	LYS	510	73.598	-3.058	5.314	1.00	43.61
ATOM	3874	CG	LYS	510	72.845	-2.306	4.632	1.00	45.46
ATOM	3875	CD	LYS	510	73.022	-2.306	3.568	1.00	54.00
ATOM	3876	CE	LYS	510	72.194	-2.912 -4.184	2.183	1.00	58.74
ATOM	3877	NZ	LYS	510	72.194	-5.323	2.007	1.00	59.63
ATOM	3881	C	LYS	510	74.065	-1.359	2.815 6.450	1.00	61.62
ATOM	3882	0	LYS	510	73.566	-1.898	7 439	1.00	42.05
ATOM	3883	N	VAL	511	74.185	-0.038	6.333	1.00	41.29
ATOM	3885	CA	VAL	511	73.719	0.894			40.14
			T		13.113	0.034	7.359	1.00	35.38

ATOM	3886	CB	VAL	511	74.932	1.554	8.074	1.00	33.16
ATOM	3887	CG1	VAL	511	75.761	0.501	8.795	1.00	29.24
ATOM	3888	CG2	VAL	511	75.804	2.295	7.054	1.00	30.37
MOTA	3889	С	VAL	511	72.856	2.005	6.776	1.00	33.90
MOTA	3890	0	VAL	511	72.722	2.110	5.558	1.00	32.53
ATOM	3891	N	ALA	512	72.261	2.813	7.655	1.00	31.97
ATOM	3893	CA	ALA	512	71.434	3.956	7.248	1.00	31.10
MOTA	3894	CB	ALA	512	70.088	3.945	7.952	1.00	27.38
ATOM	3895	C	ALA	512	72.225	5.186	7.660	1.00	30.49
ATOM	3896	0	ALA	512	72.775	5.235	8.766	1.00	30.10
ATOM	3897	N	VAL	513	72.312	6.162	6.765	1.00	30.50
ATOM	3899	CA	VAL	513	73.064	7.382	7.041	1.00	29.68
ATOM	3900	CB	VAL	<b>51</b> 3	74.204	7.593	6.015	1.00	28.89
ATOM	3901	CG1	VAL	513	74.966	8.856	6.334	1.00	26.30
MOTA	3902	CG2	VAL	513	75.134	6.389	5.987	1.00	26.66
MOTA	3903	C	VAL	513	72.171	8.607	7.012	1.00	28.50
MOTA	3904	0	VAL	513	71.536	8.893	5.994	1.00	26.27
ATOM	3905	N	LYS	514	72.091	9.282	8.154	1.00	29.18
ATOM	3907	CA	LYS	514	71.307	10.508	8.295	1.00	31.52
ATOM	3908	CB	LYS	514	70.797	10.659	9.728	1.00	33.52
ATOM	3909	CG	LYS	514	69.890	9.540	10.198	1.00	
ATOM	3910	CD	LYS	514	69.439	9.831	11.618	1.00	44.89
MOTA	3911	CE	LYS	514	68.313	8.909	12.060	1.00	51.12
ATOM	3912	NZ	LYS	514	67.029	9.137	11.307	1.00	57.11
ATOM	3916	С	LYS	514	72.233	11.681	7.956	1.00	30.75
ATOM	3917	0	LYS	514	73.390	11.698	8.379	1.00	30.08
MOTA	3918	N	MET	51.5	71.724	12.651	7.201	1.00	29.45
ATOM	3920	CA	MET	515	72.511	13.814	6.786	1.00	28.74
ATOM	3921	CB	MET	515	73.342	13.466	5.552	1.00	27.72
ATOM	3922	CG	MET	515	72.487	13.034	4.378	1.00	31.56
ATOM	3923	SD	MET	515	73.442	12.549	2.945	1.90	34.98
MOTA	3924	CE	MET	515	73.730	10.878	3.330	1.00	31.23
MOTA	3925	C	MET	515	71.585	14.966	6.444	1.00	27.75
MOTA	3926	0	MET	515	70.369	14.794	6.359	1.00	29.07
MOTA	3927	N	LEU	516	72.152	16.145	6.247	1.00	28.33
ATOM	3929	CA	LEU	516	71.348 .	17.313	5.912	1.00	31.16
ATOM	3930	CB	LEU	516	72.052	18.605	6.339	1.00	28.70
ATOM	3931	CG	LEU	516	72.312	18.866	7.826	1.00	28.33
ATOM	3932	CD1	LEU	516	73.098	20.156	7.949	1.00	28.45
MOTA	3933	CD2	LEU	516	71.020	18.959	8.604	1.00	21.64
MOTA	3934	С	LEU	516	71.069	17.378	4.421	1.00	33.22
MOTA	3935	0	LEU	516	71.762	16.760	3.619	1.00	35.00
ATOM	3936	N	LYS	517	70.022	18.100	4.061	1.00	34.69
ATOM	3938	CA	LYS	517	69.696	18.286	2.665	1.00	34.20
ATOM	3939	CB	LYS	517	68.194	18.475	2.496	1.00	37.45
ATOM	3940	CG	LYS	517	67.403	17.264	2.950	1.00	43.71
MOTA	3941	CD	LYS	517	66.157	17.072	2.126	1.00	51.25
ATOM	3942	CE	LYS	517	65.123	18.135	2.419	1.00	58.56
MOTA	3943	NZ	LYS	517	64.010	18.049	1.438	1.00	63.12
MOTA	3947	С	LYS	517	70.482	19.533	2.259	1.00	33.81
ATOM	3948	0	LYS	517	70.991	20.244	3.130	1.00	33.17
ATOM	3949	N	SER	518	70.603	19.788	0.959	1.00	33.42
ATOM	3951	CA	SER	518	71.369	20.938	0.472	1.00	33.33
MOTA	3952	CB	SER	518	71.550	20.842	-1.042	1.00	33.23

MOTA	3953	OG	SER	518	70.306	20.624	-1.678	1.00	38.84
ATOM	3955	C	SER	518	70.794	22.298	0.846	1.00	33.23
ATOM	3956	0	SER	518	71.509	23.305	0.865	1.00	34.14
MOTA	3957	N	ASP	519	69.510	22.313	1.178	1.00	32.77
ATOM	3959	CA	ASP	519	68.825	23.541	1.570	1.00	33.26
MOTA	3960	СВ	ASP	519	67.401	23.563	0.995	1.00	35.10
ATOM	3961	CG	ASP	519	66.484	22.503	1.617	1.00	38.98
ATOM	3962	OD1	ASP	519	66.958	21.430	2.042	1.00	
ATOM	3963	OD2	ASP	519	65.261	22.754	1.674	1.00	37.30
ATOM	3964	С	ASP	519	68.793	23.747	3.091	1.00	43.65
ATOM	3965	0	ASP	519	68.114	24.648	3.580	1.00	33.05
ATOM	3966	N	ALA	520	69.538	22.931	3.833		35.19
ATOM	3968	CA	ALA	520	69.570	23.032	5.293	1.00	31.38
ATOM	3969	CB	ALA	520	70.264	21.830	5.870	1.00	29.47
MOTA	3970	С	ALA	520	70.229	24.301	5.812	1.00	29.74
ATOM	3971	0	ALA	520	71.004	24.952	5.106	1.00	29.83
MOTA	3972	N	THR	521	69.938	24.616		1.00	30.23
ATOM	3974	CA	THR	521	70.487	25.793	7.071	1.00	31.57
ATOM	3975	СВ	THR	521	69.361	26.736	7.742	1.00	34.56
ATOM	3976	OG1	THR	521	68.670	26.736	8.302	1.00	38.37
ATOM	3978	CG2	THR	521	68.357		9.376	1.00	41.75
ATOM	3979	C	THR	521	71.353	27.117	7.209	1.00	38.30
ATOM	3980	Ö	THR	521	71.333	25.363	8.916	1.00	33.22
ATOM	3981	N	GLU	522	72.092	24.207	9.327	1.00	32.31
ATOM	3983	CA	GLU	522	72.951	26.310 26.042	9.479	1.00	34.43
ATOM	3984	CB	GLU	522	73.634		10.619	1.00	39.53
ATOM	3985	CG	GLU	522	74.398	27.340 27.271	11.068	1.00	46.35
ATOM	3986	CD	GLU	522	75.772		12.402	1.00	58.03
ATOM	3987	OE1	GLU	522	76.800	26.603 27.321	12.301	1.00	63.14
ATOM	3988	QE2	GLU	522	75.824		12.404	1.00	61.75
ATOM	3989	C	GLU	522	72.130	25.359	12.158	1.00	66.35
ATOM	3990	C	GLU	522	72.642	25.428	11.765	1.00	38.40
ATOM	3991	N	LYS	523	70.853	24.622 25.792	12.543	1.00	37.92
ATOM	3993	CA	LYS	523	69.995	25.261	11.849	1.00	36.43
ATOM	3994	CB	LYS	523	68.703	26.065	12.893	1.00	36.83
ATOM	3995	CG	LYS	523	67.793	25.636	13.008	1.00	40.88
ATOM	3996	CD	LYS	523	66.584	24.898	14.152	1.00	44.55
MOTA	3997	CE	LYS	523	65.629		13.607	1.00	52.68
ATOM	3998	NZ	LYS	523	64.537	24.483	14.708	1.00	56.04
ATOM	4002	C	LYS	523	69.689	23.646 23.804	14.123	1.00	58.13
ATOM	4003	ō	LYS	523	69.645		12.601	1.00	35.27
ATOM	4004	N	ASP	524	69.496	22.985	13.513	1.00	36.58
ATOM	4006	CA	ASP	524	69.235	23.473	11.326	1.00	32.27
ATOM	4007	CB	ASP	524		22.089	10.963	1.00	27.18
ATOM	4008	CG	ASP	524	68.952	21.953	9.480	1.00	26.32
ATOM	4009	OD1	ASP		67.635	22.555	9.089	1.00	25.22
ATOM	4010	OD2	ASP	524	66.662	22.394	9.848	1.00	31.78
ATOM	4011	C	ASP	524	67.568	23.190	8.028	1.00	24.00
ATOM	4012			524	70.445	21.268	11.342	1.00	26.83
ATOM	4012	0 N	ASP	524	70.312	20.165	11.851	1.00	28.65
ATOM	4015	CA	LEU	525	71.633	21.827	11.129	1.00	28.69
ATOM	4015	CB	LEU	525	72.872	21.148	11.473	1.00	26.96
ATOM	4017		LEU	525	74.077	21.981	11.049	1.00	22.80
ATOM		CG	LEU	525	75.445	21.355	11.341	1.00	22.32
ALON	4018	CD1	LEU	525	75.522	19.883	10.858	1.00	18.89

ATOM	4019	CD2	LEU	<b>5</b> 25	76.504	22.212	10.704	1.00	17.44
ATOM	4020	C	LEU	525	72.886	20.926	12.980	1.00	28.00
ATOM	4021	0	LEU	525	73.160	19.816	13.462	1.00	28.82
ATOM	4022	N	SER	526	72.567	21.992	13.707	1.00	27.98
ATOM	4024	CA	SER	526	72.496	21.994	15.168	1.00	30.78
ATOM	4025	CB	SER	526	71.939	23.345	15.627	1.00	33.18
ATOM	4026	OG	SER	526	71.624	23.347	17.009	1.00	42.73
ATOM	4028	С	SER	526	71.599	20.865	15.704	1.00	30.56
ATOM	4029	0	SER	526	71.906	20.206	16.716	1.00	31.92
ATOM	4030	И	ASP	527	70.484	20.665	15.018	1.00	28.19
ATOM	4032	CA	ASP	527	69.516	19.651	15.366	1.00	27.41
ATOM	4033	CB	ASP	527 527	68.207	19.932	14.632	1.00	27.63
ATOM	4034	CG	ASP	527	67.492	21.172	15.149	1.00	27.37
ATOM ATOM	4035 4036	OD1 OD2	ASP ASP	527 527	67.870	21.728	16.211	1.00	26.70
ATOM	4037	C C	ASP	527 527	66.525	21.579	14.487	1.00	33.80
ATOM	4037	0	ASP	52 <i>7</i> 527	70.007 69.722	18.241 17.309	15.063 15.816	1.00	27.36
ATOM	4039	N.	LEU	528	70.716	18.077	13.952	1.00	30.13
ATOM	4041	CA	LEU	528	71.245	16.765	13.588	1.00	25.76 25.29
ATOM	4042	CB	LEU	528	71.777		12.143	1.00	23.65
ATOM	4043	CG	LEU	528	72.283	15.432	11.574	1.00	25.86
ATOM	4044	CD1	LEU	528	71.234	14.341	11.770	1.00	23.35
ATOM	4045	CD2	LEU	528	72.652	15.566	10.102	1.00	17.46
MOTA	4046	c	LEU	528	72.351	16.368	14.578	1.00	25.66
MOTA	4047	С	LEU	528	72.418	15.210	15.015	1.00	24.02
ATOM	4048	N	ILE	529	73.200	17.338	14.934	1.00	26.36
ATOM	4050	CA	ILE	529	74.304	17.130	15.886	1.00	26.17
ATOM	4051	CB	ILE	529	75.192	18.381	16.003	1.00	22.72
ATOM	4052	CG2	ILE	529	76.250	18.180	17.057	1.00	21.32
ATOM	4053	CG1	ILE	529	75.876	18.666	14.685	1.00	20.71
MOTA	4054	CD1	ILE	529	76.621	19.965	14.675	1.00	25.60
MOTA	4055	C	ILE	529	73.756	16.835	17.283	1.00	29.87
ATOM	4056	၁	ILE	529	74.253	15.948	1.7.977	1.00	32.20
ATOM	4057	N	SER	530	72.741	17.591	17.693	1.00	28.63
ATOM	4059	CA	SER	530	72.143	17.381	18.991	1.00	32.21
ATOM	4060	CB	SER	530	71.031	18.399	19.231	1.00	37.45
ATOM	4061	OG	SER	530	70.065	18.342	18.195	1.00	49.52
ATOM	4063	C	SER	530	71.598	15.956	19.075	1.00	30.96
ATOM ATOM	4064 4065	O N	SER GLU	530	71.728	15.301	20.105	1.00	33.05
ATOM	4067	ÇA	GLU	531 531	70.996 70.468	15.476	17.996	1.00	29.13
ATOM	4068	CB	GLU	531	69.672	14.117	17.987	1.00	29.84
ATOM	4069	CG	GLU	531	69.093	13.847	16.709	1.00	30.29
ATOM	4070	CD	GLU	531	68.521	12.445	16.666	1.00	27.39
ATOM	4071	OE1	GLU	531	67.929	12.074 10.981	15.331 15.228	1.00	31.34
ATOM	4072	OE2	GLU	531	68.660	12.860	14.376	1.00	35.90
ATOM	4073	C	GLU	531	71.600	13.081	18.109	1.00	38.37 28.48
ATOM	4074	0	GLU	531	71.468	12.094	18.822	1.00	28.48
ATOM	4075	N	MET	532	72.682	13.281	17.364	1.00	
ATOM	4077	CA	MET	532	73.832	12.376	17.409	1.00	28.12 27.64
ATOM	4078	CB	MET	532	74.953	12.899	16.499	1.00	26.47
ATOM	4079	CG	MET	532	76.267	12.125	16.601	1.00	22.25
ATOM	4080	SD	MET	532	77.406	12.610	15.286	1.00	30.32
ATOM	4081	CE	MET	532	77.613	14.366	15.661	1.00	20.92
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ATO	_	_	ME	r 532	74.339	12.328	8 18.83	2 1.00	) ) 7 0 ~	
ATO			ME	r 532	74.640	11.26		•		
ATO			GL	J 533	74.439	13.49				
ATO			GLU	J 533	74.906	13.594				
ATO			GLU	533	75.071	15.064		_		
ATO			GLU	533	76.216	15.745				
ATO			GLU	533	77.564	15.070		•		
ATON			L GLU	533	78.001	14.969				
ATON			2 GLU	533	78.202	14.643				
ATON		_	GLU	533	73.981	12.850				
ATOM			GLU	533	74.455	12.093				
ATOM			MET	534	72.670	13.014				
ATOM			MET	534	71.692	12.346			29.70	
ATOM			MET	534	70.258	12.751			27.97	
ATOM			MET	534	69.311	12.594	23.278	1.00	28.95	
ATOM			MET	534	67.538	12.682	22.961	0.50	29.62	
ATOM			MET	534	67.269	14.452	22.795	0.50	29.87	
ATOM		С	MET	534	71.855	10.821	22.362	0.50	31.07	PRT1
ATOM		0	MET	534	71.833	10.143	23.386	1.00	28.36	
ATOM		N	MET	535	72.048	10.297		1.00	27.02	
ATOM		CA	MET	535	72.239	8.861	21.151	1.00	26.96	
ATOM	4106	CB	MET	535	72.347	8.521	20.947	1.00	26.63	
ATOM	4107	CG	MET	535	71.089	8.778	19.456	1.00	24.67	
ATOM	4108	SD	MET	535	71.160	8.062	18.659	1.00	23.15	
ATOM	4109	CE	MET	535	71.251	9.486	17.011	1.00	24.57	
ATOM	4110	C	MET	535	73.498	8.390	16.023	1.00	24.79	
ATOM	4111	0	MET	535	73.564	7.259	21.669	1.00	27.66	
ATOM	4112	N	LYS	536	74.515	9.246	22.164	1.00	28.83	
ATOM	4114	CA	LYS	536	75.757		21.698	1.00	29.13	
MOTA	4115	СВ	LYS	536	76.812	8.918	22.392	1.00	30.50	•
ATOM	4116	CG	LYS	536	77.499	9.985	22.131	1.00	29.15	
ATOM	4117	CD	LYS	536	78.377	9.883 11.100	20.802	1.00	27.71	
ATOM	4118	CE	LYS	536	79.085	11.096	20.615	1.00	28.12	
ATOM	4119	NZ	LYS	536	79.688	12.436	19.279	1.00	26.89	
ATOM	4123	С	LYS	536	75.480	8.836	19.077	1.00	27.54	
ATOM	4124	0	LYS	536	75.921	7.908	23.892	1.00	31.92	
ATOM	4125	N	MET	537	74.742	9.814	24.559	1.00	31.19	
ATOM	4127	CA	MET	537	74.384	9.881	24.409	1.00	34.02	
ATOM	4128	CB	MET	537	73.648	11.197	25.822	1.00	36.35	
ATOM	4129	CG	MET	53 <i>7</i>	73.096	11.376	26.083	1.00	43.33	
ATOM	4130	SD	MET	537	71.426	10.674	27.507	1.00	54.60	
ATOM	4131	CE	MET	537	71 684	9.813	27.856	1.00	67.38	
ATOM	4132	C	MET	537	73.507	8.705	29.440	1.00	62.03	
ATOM	4133	0	MET	537	73.744		26.253	1.00	34.53	
MOTA	4134	N	ILE	538	72.496	8.069	27.275	1.00	36.76	
ATOM	4136	CA	ILE	538	71.568	8.425	25.454	1.00	32.24	
MOTA	4137	CB	ILE	538	70.396	7.367	25.757	1.00	29.88	
ATOM	4138	CG2	ILE	538		7.384	24.757	1.00	26.98	
ATOM	4139	CG1	ILE	538	69.582	6.096	24.842	1.00	27.93	
ATOM	4140	CD1	ILE	538	69.527	8.614	25.036	1.00	22.58	
ATOM	4141	C		538	68.399	8.787	24.058		24.58	
ATOM	4142	0		538 538	72.236	6.006	25.804		31.83	
ATOM	4143	N		536 539	71.983	5.227	26.713		36.32	
ATOM	4145	CA			73.102		24.848	1.00	32.45	
			JD 1	539	73.744	4.422	24.850	1.00	32.13	
CCCD II-										

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F	MOTA	4146	С	GLY	539	72.974	3.380	24.056	1.00	33.83
7	MOTA	4147	0	GLY	539	71.876	3.654	23.530	1.00	33.75
P	MOTA	4148	N	LYS	540	73.539	2.173	24.010	1.00	33.36
A	MOTA	4150	CA	LYS	540	72.980	1.054	23.256	1.00	37.04
A	MOTA	4151	CB	LYS	540	74.110	0.181	22.709	1.00	39.21
A	MOTA	4152	CG	LYS	540	74.865	0.893	21.623	1.00	48.72
A	MOTA	4153	CD	LYS	540	75.818	0.009	20.850	1.00	56.84
A	MOT	4154	CE	LYS	540	76.225	0.693	19.516	1.00	62.14
Ά	MOT	4155	NZ	LYS	540	77.252	-0.102	18.805	1.00	71.02
A	MOT	4159	C	LYS	540	71.938	0.162	23.901	1.00	36.51
A	MOT	4160	0	LYS	540 .	71.963	-0.096	25.113	1.00	38.52
A	TOM	4161	N	HIS	541	71.017	-0.295	23.058	1.00	32.98
A	TOM	4163	CA	HIS	541	69.963	-1.230	23.424	1.00	31.20
Α	TOM	4164	CB	HIS	541	68.779	-0.561	24.095	1.00	30.35
A	TOM	4165	CG	HIS	541	67.815	-1.540	24.694	1.00	32.56
A	MOT	4166	CD2	HIS	541	67.737	-2.058	25.941	1.00	32.45
A	MOT	4167	ND1	HIS	541	66.795	-2.124	23.974	1.00	29.22
A.	MOT	4169	CE1	HIS	541	66.134	-2.965	24.753	1.00	31.56
A	MOT	4170	NE2	HIS	541	66.679	-2.932	25.957	1.00	32.22
Α	MOT.	4172	С	HIS	541	69.509	-1.937	22.152	1.00	32.00
A	MOT	4173	O	HIS	541	69.409	-1.324	21.095	1.00	32.84
A	TOM	4174	N	LYS	542	69.187	-3.222	22.273	1.00	33.61
A	MOT	4176	CA	LYS	542	68.786	-4.061	21.154	1.00	31.54
	MOT	4177	C.B	LYS	542	68.653	-5.516	21.596	1.00	33.94
	TOM	4178	CG	LYS	542	6.8.322	-6.451	20.437	1.00	42.34
A	MOT	4179	CD	LYS	542	68.083	-7.885	20.856	1.00	47.57
	TOM	4180	CE	LYS	542	67.634	-8.726	19.658	1.00	52.70
	TOM	4181	NZ	LYS	542	67.402	-10.146	20.023	1.00	59.51
	TOM	4185	C	LYS	542	67.495	-3.611	20.487	1.00	29.57
	TOM	4186	0	LYS	542	67.268	-3.884	19.305	1.00	27.99
	TOM	4187	N	ASN	543	66.649	-2.931	21.253	1.00	28.32
	TOM	4189	CA	ASN	543	65.378	-2.476	20.714	1.00	28.86
	TOM	4190	CB	ASN	543	64.231	-2.947	21.601	1.00	29.33
	TOM	4191	CG	ASN	543	64.247	-4.452	21.811	1.00	29.64
	TOM	4192	OD1	ASN	543	64.437	-4.926	22.930	1.00	33.86
	TOM	4193	ND2	ASN	543	64.106	-5.206	20.732	1.00	28.02
	TOM	4196	C	ASN	543	65.252	-0.983	20.378	1.00	29.69
	TOM	4197	0	ASN	543	64.159	-0.413	20.457	1.00	30.02
	TOM	4198	N	ILE	544	66.372	-0.357	20.011	1.00	27.35
	TOM	4200	CA	ILE	544	66.382	1.046	19.593	1.00	25.95
	TOM	4201	CB	ILE	544	66.898	2.030	20.706	1.00	25.56
	TOM	4202 4203	CG2	ILE	544	66.148	1.819	22.037	1.00	21.06
	TOM		CG1	ILE	544	68.406	1.901	20.902	1.00	25.61
	TOM	4204	CD1	ILE	544	68.952	2.818	21.976	1.00	25.89
	TOM	4205	C	ILE	544	67.341	1.083	18.399	1.00	25.97
	TOM	4206	0	ILE	544	68.126	0.152	18.227	1.00	25.69
	TOM	4207	N	ILE	545	67.226	2.095	17.537	1.00	27.27
	TOM	4209	CA	ILE	545	68.129	2.243	16.384	1.00	27.02
	TOM	4210	CB	ILE	545	67.541	3.194	15.307	1.00	27.30
		4211	CG2	ILE	545	68.592	3.553	14.269	1.00	26.52
	TOM	4212	CG1	ILE	545	66.309	2.570	14.638	1.00	22.63
	TOM	4213	CD1	ILE	545	66.605	1.447	13.665	1.00	17.57
	TOM	4214	C	ILE	545	69.383	2.873	16.979	1.00	28.55
A	TOM	4215	0	ILE	545	69.346	4.014	17.451	1.00	29.47

ATO			AS.	N 546	70.48	2 2.12	3 16 00		_
ATO			AS	N 546	71.748				
ATC		19 CB	AS	N 546	72.49				
ATC		50 CG	ASI	V 546	71.732				
ATC		21 OD	1 ASI		71.580	- •			·
ATO		22 ND:	2 ASI		71.267				
ATO		?5 C	ASN		72.700	51			
ATO		6 0	ASN		72.679				_
ATO		7 N	LEU		73.543	•			
ATO	M 422	9 CA	LEU		74.570				32.29
ATO		0 CB	LEU		75.043				30.93
ATO	M 423	1 CG	LEU		76.075	6.076			
ATO		2 CD1			75.553	7.088			22.12
ATON	M 423	3 CD2				7.815		1.00	22.10
ATON	423	4 C'	LEU		76.415	8.089		1.00	18.67
ATOM	423	5 0	LEU		75.756	4.039		1.00	30.70
ATOM	4236	5 N	LEU	548	76.284	3.361		1.00	34.46
ATOM	1 4238	3 CA	LEU	548	76.141	3.993		1.00	30.97
ATOM	1 4239	Э СВ	LEU	548	77.262	3.165	_	1.00	30.73
ATOM	4240	) CG	LEU	548	76.929	2.406	13.281	1.00	29.24
ATOM	4241		LEU	548	75.788	1.394	13.371	1.00	28.77
ATOM	4242		LEU	548	75.924	0.460	12.209	1.00	26.55
ATOM	4243		LEU	548	75.839	0.616	14.683	1.00	23.48
ATOM	4244		LEU	548	78.522	3.982	14.347	1.00	33.00
ATOM			GLY	549	79.640	3.500	14.558	1.00	35.92
ATOM	4247		GLY	549	78.351	5.215	13.901	1.00	32.52
ATOM	4248		GLY	549	79.503	6.051	13.673	1.00	32.76
ATOM	4249	0	GLY	549	79.092	7.411	13.180	1.00	33.72
ATOM	4250	N	ALA	550	77.895	7.707	13.092	1.00	35.01
ATOM	4252	CA	ALA	550	80.089	8.226	12.840	1.00	33.47
MOTA	4253	CB	ALA	550	79.848	9.566	12.337	1.00	30.69
ATOM	4254	C	ALA	550	79.555	10.509	13.497	1.00	28.66
MOTA	4255	0	ALA	550	81.022	10.099	11.523	1.00	30.41
ATOM	4256	N	CYS	551	82.181	9.780	11.808	1.00	25.13
ATOM	4258	CA	CYS	551	80.695	10.817	10.446	1.00	30.29
ATOM	4259	CB	CYS	551	81.675	11.490	9.584	1.00	28.44
MOTA	4260	SG	CYS	551	81.432	11.214	8.096	1.00	27.25
ATOM	4261	C	CYS	551	81.639	9.508	7.566	1.00	28.89
ATOM	4262	0	CYS	551	81.337	12.950	9.883	1.00	27.07
ATOM	4263	N	THR	552	80.293	13.441	9.467	1.00	29.86
ATOM	4265	CA	THR	552	82.184	13.616	10.658	1.00	25.10
ATOM	4266	CB	THR	552	81.952	14.997	11.047	1.00	24.37
ATOM	4267	OG1	THR	552 552	81.959	15.091	12.569	_	27.67
MOTA	4269	CG2	THR	552	83.271	14.760	13.052		26.11
ATOM	4270	C		552 552	80.951	14.120	13.164		30.41
ATOM	4271	0	_		83.003	15.980		_	24.51
ATOM	4272			552	82.804	17.194	10.604		21.56
ATOM	4274			553	84.151	15.441			27.13
ATOM	4275			553	85.284	16.243			26.64
ATOM	4276			553	86.592	15.679			25.24
ATOM	4277			553	86.641	15.561			22.38
ATOM	4278			553	86.464				24.04
ATOM	4279			553	87.267	17.815			31.50
ATOM	4282			553	85.403				21.59
	4404	C	GLN !	553	85.384	16.276			28.02
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ATOM	4283	0	GLN	553	85.069	15.293	7.537	1.00	30.20
ATOM	4284	N	ASP	554	85.794	17.430	7.695	1.00	28.08
ATOM	4286	CA	ASP	554	86.000	17.652	6.263	1.00	30.14
ATOM	4287	CB	ASP	554	87.330	17.034	5.833	1.00	29.82
MOTA	4288	CG	ASP	554	88.451	17.470	6.707	1.00	31.79
ATOM	4289	OD1	ASP	554	88.699	18.666	6.767	1.00	36.45
MOTA	4290	OD2	ASP	554	89.066	16.623	7.364	1.00	33.06
ATOM	4291	C	ASP	554	84.895	17.217	5.317	1.00	29.52
MOTA	4292	0	ASP	554	85.128	16.411	4.424	1.00	33.67
ATOM	4293	N	GLY	555	83.709	17.793	5.488	1.00	29.02
MOTA	4295	CA	GLY	555	82.586	17.476	4.621	1.00	26.05
ATOM	4296	C	GLY	555	81.286	17.447	5.405	1.00	23.80
ATOM	4297	0.	GLY	555	81.269	17.751	6.597	1.00	24.09
ATOM	4298	Ŋ	PRO	556	80.175	17.117	4.740	1.00	23.29
ATOM	4299	CD	PRO	556	80.094	16.804	3.304	1.00	18.93
ATOM	4300	CA	PRO	556	78.860	17.045	5.378	1.00	23.45
MOTA	4301	CB	PRO	556	77.943	16.643	4.226	1.00	22.35
ATOM	4302	CG	PRO	556	78.889	15.931	3.261	1.00	24.94
ATOM	4303	С	PRO	556	78.806	16.019	6.503	1.00	26.66
ATOM	4304	0	PRO	556	79.488	14.984	6.464	1.00	27.76
ATOM	4305	N	LEU	557	78.006	16.324	7.522	1.00	29.14
ATOM	4307	CA	LEU	557	77.842	15.440	8.676	1.00	30.83
ATOM	4308	CB	LEU	557	77.173	16.181	9.842	1.00	28.40
ATOM ATOM	4309 4310	CG CD1	LEU	557	76.775	15.393	11.097	1.00	22.93
ATOM	4311	CD1	LEU	557 557	77.989	14.897	11.835	1.00	23.02
ATOM	4312	C	LEU	557	75.970 77.028	16.285	11.984	1.00	23.53
MOTA	4313	0	LEU	557	75.968	14.200 14.293	8 321 7.694	1.00 1.00	31.04
ATOM	4314	N	TYR	558	77.552	13.041	8.700	1.00	31.89 29.88
ATOM	4316	CA	TYR	558	76.891	11.773	8.460	1.00	27.80
MOTA	4317	СВ	TYR	558	77.741	10.978	7.562	1.00	28.04
ATOM	4318	CG	TYR	558	77.895	11.339	6.122	1.00	29.98
ATOM	4319	CD1	TYR	558	78.843	10.751	5.289	1.00	31.81
ATOM	4320	CE1	TYR	558	78.980	11.140	3.956	1.00	32.22
MOTA	4321	CD2	TYR	558	77.086	12.335	5.584	1.00	31.50
ATOM	4322	CE2	TYR	558	77.214	12.729	4.256	1.00	31.57
ATOM	4323	CZ	TYR	558	78.166	12.125	3.449	1.00	32.04
ATOM	4324	OH	TYR	558	78.317	12.511	2.134	1.00	33.34
ATOM	4326	C	TYR	558	76. <b>7</b> 15	11.099	9.809	1.00	27.34
ATOM	4327	0	TYR	558	. 77.678	10.937	10.558	1.00	25.80
ATOM	4328	N	VAL	559	75.464	10.798	10.147	1.00	28.06
ATOM	4330	CA	VAL	559	75.118	10.118	11.394	1.00	26.67
ATOM	4331	CB	VAL	559	73.930	10.816	12.129	1.00	26.22
ATOM	4332	CG1	VAL	559	73.590	10.079	13.425	1.00	22.58
ATOM	4333	CG2	VAL	559	74.298	12.278	12.440	1.00	23.09
ATOM ATOM	4334	C	VAL	559	74.745	8.715	10.943	1.00	24.32
ATOM	4335 4336	0	VAL	559	73.665	8.464	10.412	1.00	26.37
ATOM		N	ILE	560 560	75.689	7.815	11.095	1.00	23.63
ATOM	4338	CA	ILE		75.514	6.448	10.664	1.00	24.67
ATOM	4339 4340	CB CG2	ILE ILE	560 560	76.901	5.859	10.299	1.00	24.62
ATOM	4341	CG2	ILE	560	76.753 77.627	4.507	9.646	1.00	30,13
ATOM	4342	CD1	ILE	560	77.627 79.114	6.810	9.326	1.00	21.87
ATOM	4343	C	ILE	560	74.814	6.538 5.621	9.162 11.737	1.00	22.25
		-		200	,4.014	J. 021	11.131	1.00	27.30

ימ	rom .		_							
		4344	0	ILE	560	75.30	06 5.50	ns 12 a		
		1345	N	VAL	561					
		1347	CA	VAL	561	72.89				
		1348	CB	VAL	561	71.57				0 26.16
		349	CG1	VAL		71.86				
		350	CG2	VAL		70.67				0 24.11
AT	OM 4	351	С	VAL	561					
AT	OM 4	352	0	VAL	561	72.57			51 1.0	
AT	OM 4	353	N	GLU	562	72.85			34 1.00	
AT	OM 4	355	CA	GLU		71.99		9 12.59		
ATO		356	CB		562	71.60		5 12.21		-4.00
ATO		357		GLU	562	71.09		8 13.44		~
ATO		_		GLU	562	72.17	0 -0.39			-5.00
ATC				GLU	562	71.643	-0.969			
ATC				GLU	562	72.389	-1.714		· - <del>-</del>	
ATO				GLU	562	70.491		-		
				<b>GLU</b>	562	70.529				
ATO			О (	GLU	562	69.581				29.67
ATO			4 ;	ľYR	563	70.666		_		32.53
ATO		65 (	A :	ľYR	563	69.699				30.70
ATO			B j	YR	563	70.419				30.65
ATO		67 (	:G 1	YR	563	69.510				30.83
ATO		68 C	_	YR	563					32.10
ATO	430			YR	563	68.545		6.235	1.00	33.24
NOTA		70 C		YR	563	67.715	-	5.160	1.00	34.65
ATON	431		_	YR	563	69.609	-2.098	5.922	1.00	31.04
ATOM	1 437		_	YR		68.779	-2.353	4.838		33.12
ATOM		_		YR	563	67.831	-1.413	4.470		34.22
ATOM			_		563	67.902	~1.650	3.400		
ATOM		_	_	YR	563	68.592	.1.223	9.406		34.76
ATOM					563	68.855	~2.325	9.884	1.00	34.39
ATOM					564	67.356	-0.861	9.091		34.87
АТОМ					564	66.212	-1.726	9.324	1.00	35.49
ATOM					564	65.213	-1.000	10.210	1.00	35.41
ATOM			AI	A.	564	65.585	-2.056		1.00	35.93
ATOM	438	_	AI		564	64.789	-1.276	7.962	1.00	37.19
	438		SE	R s	65	65.931	-3.211	7.434	1.00	38.08
ATOM	4389		SE	R s	65	65.433		7.401	1.00	37.14
ATOM	4386	5 CB	SE	R 5	65	66.151	-3.616	6.080	1.00	36.83
ATOM	4387	7 OG	SE		65	66.105	-4.881	5.614	1.00	35.24
ATOM	4389	) C	SE		65	63.932	-5.873	6.619	1.00	34.96
ATOM	4390	0	SE		65	63.428	-3.782	5.886	1.00	38.65
ATOM	4391	N	LY	_	66		-3.617	4.760	1.00	37.80
ATOM	4393	CA	LY		66	63.212	-4.077	6.964		38.96
ATOM	4394	CB	LYS		66	61.772	-4.271	6.851		37.83
ATOM	4395		LYS			61.357	-5.495	7.655		39.07
ATOM	4396				66	61.954	-6. <b>76</b> 5	7.078		43.73
ATOM	4397	CE	LYS		66	61.813	-7.950	7.996		
ATOM	4398		LYS		56	62.258	-9.216	7.299		47.07
ATOM		NZ	LYS		56	62.361	-10.326	8.278		47.77
ATOM	4402	C	LYS		56	60.899	-3.050	7.165		51.48
	4403	0	LYS		6	59.702	-3.180			37.53
MOTA	4404	N	GLY	56	7	61.496	-1.866	7.442		38.55
ATOM	4406	CA	GLY	56	7	60.788	-0.627	7.066	1.00	35.23
ATOM	4407	C	GLY			60.120		7.305	1.00	33.64
ATOM	4408	0	GLY			60.518	-0.485	8.656	1.00 3	33.24
ATOM	4409	N	ASN	56			-1.133	9.627		3.80
					-	59.120	0.389			1.65
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ATOM	4411	CA	ASN	568	58.407	0.623	9.952	1.00	33.38
ATOM	4412	CB	ASN	568	57.831	2.055	10.025	1.00	37.10
MOTA	4413	CG	ASN	568	56.624	2.272	9.116	1.00	37.78
MOTA	4414	OD1	ASN	568	55.552	1.708	9.337	1.00	41.15
ATOM	4415	ND2	ASN	568	56.780	3.147	8.124	1.00	35.74
ATOM	4418	С	ASN	568	57.357	-0.435	10.263	1.00	33.33
ATOM	4419	0	ASN	568	56.917	-1.178	9.384	1.00	32.54
ATOM	4420	N	LEU	569	56.971	-0.490	11.532	1.00	33.35
MOTA	4422	CA	LEU	569	56.004	-1.455	12.040	1.00	32.38
ATOM	4423	CB	LEU	569	55.838	-1.263	13.552	1.00	27.50
ATOM	4424	CG	LEU	569	54.954	-2.259	14.291	1.00	26.34
ATOM	4425	CD1	LEU	569	55.452	-3.671	14.007	1.00	24.19
ATOM	4426	CD2	LEU	569	54.968	-1.951	15.787	1.00	21.44
ATOM	4427	С	LEU	569	54.641	-1.433	11.355	1.00	33.35
ATOM	4428	0	LEU	569	54.060	-2.484	11.095	1.00	34.99
ATOM	4429	N	ARG	570	54.130	-0.239	11.083	1.00	34.36
ATOM	4431	CA	ARG	570	52.827	-0.091	10.445	1.00	36.82
MOTA	4432	CB	ARG	570	52.548	1.393	10.188	1.00	37.28
ATOM	4433	CG	ARG	570	51.210	1.689	9.539	1.00	43.90
ATOM	4434	CD	ARG	570	51.212	3.099	8.967	1.00	50.39
ATOM	4435	NE	ARG	570	52.273	3.268	7.973	1.00	54.99
ATOM	4437	CZ	ARG	570	53.075	4.328	7.887	1.00	54.96
MOTA	4438	NH1	ARG	570	52.947	5.343	8.735	1.00	54.71
ATOM	4441	NH2	ARG	570	54.030	4.357	6.966	1.00	56.12
ATOM	4444	C	ARG	570	52.818	~0.877	9.133	1.00	36.53
ATOM	4445	0	ARG	570	51.968	-1.737	8.909	1.00	34.68
ATOM	4446	N	GLU	571	53.830	-0.611	8.320	1.00	37.14
ATOM	4448	CA	GLU	571	53.954	-1.253	7.031	1.00	37.94
MOTA	4449	СВ	GLU	571	55.126	-0.558	5.274	1.00	39.71
ATOM	4450	CG	GLU	571	54.834	0.916	6.062	1.00	44.69
ATOM	4451	CD	GLU	571	55.934	1.665	5.346	1.00	52.22
MOTA	4452	OE1	GLU	571	57.098	1.196	5.358	1.00	54.87
MOTA	4453	OE2	GLU	571	55.629	2.743	4.777	1.00	56.37
MOTA	4454	C	GLU	571	54.258	-2.744	7.164	1.00	36.53
ATOM	4455	0	GLU	571	53.692	-3.550	6.426	1.00	36.35
MOTA	4456	N	TYR	572	55.105	-3.105	8.120	1.00	35.77
ATOM	4458	CA	TYR	572	55.456	-4.499	8.371	1.00	36.28
MOTA	4459	CB	TYR	572	56.446	-4.555	9.534	1.00	30.27
ATOM	4460	CG	TYR	572	56.859	-5.925	10.006	1.00	31.65
ATOM	4461	CD1	TYR	572	57.889	-6.626	9.371	1.00	29.40
ATOM	4462	CE1	TYR	572	58.354	-7.839	9.883	1.00	29.32
MOTA.	4463	CD2	TYR	572	56.292	-6.480	11.161	1.00	35.17
ATOM	4464	CE2	TYR	572	56.749	-7.696	11.680	1.00	33.08
MOTA	4465	CZ	TYR	572	57.780	-8.366	11.038	1.00	35.15
ATOM	4466	OH	TYR	572	58.234	-9.559	11.558	1.00	36.91
ATOM	4468	С	TYR	572	54.189	-5.321	8.672	1.00	37.70
MOTA	4469	0	TYR	572	53.942	-6.369	8.068	1.00	36.82
ATOM	4470	N	LEU	573	53.368	-4.799	9.576	1.00	37.64
MOTA	4472	CA	LEU	573	52.126	-5.442	9.970	1.00	36.03
MOTA	4473	СВ	LEU	573	51.497	-4.659	11.122	1.00	36.17
MOTA	4474	CG	LEU	573	52.257	-4.641	12.445	1.00	36.39
ATOM	4475	CD1	LEU	573	51.590	-3.665	13.412	1.00	36.17
ATOM	4476	CD2	LEU	573	52.311	-6.042	13.032	1.00	32.13
MOTA	4477	C	LEU	573	51.117	-5.562	8.822	1.00	36.33

							2	00				
A	TOM 4	478	0	LEU	573							
A'	TOM 4	479		GLN	574			-6.		649	1.00	35.19
A'	TOM 4	481		GLN				-4.5		038	1.00	
A	TOM 4			GLN	574			-4.5	514 6.	936	1.00	41.78
A					574			-3.1		413	1.00	
				GLN	574	48.8		-2.2		264	1.00	43.82
				GLN	574	48.8		-0.8		801		45.42
				GLN	574	49.4	56	-0.5		772	1.00	49.56
			_	<b>JLN</b>	574	48.2	07	0.0			1.00	52.22
AT		`		SLN	574	50.4	01	-5.4			1.00	54.86
AT		190	_	SLN	574	49.5		-5.8			1.00	42.89
AT		91 N	-	LA	575	51.69		-5.6			1.00	46.15
				LA	575	52.16					1.00	42.39
ATO			B A	LA	575	53.59		-6.5			1.00	40.19
AT(		95 C	A	LA	575	52.08		-6.16			1.00	40.68
ATO		96 O	A	LA	575			-7.97			1.00	40.49
ATC	DM 44	97 N		RG	576	52.43		-8.86			1.00	43.34
ATC	M 44	99 C.		RG	576	51.63		-8.19			.00	38.76
ATO	M 450		_	RG		51.53		-9.54			.00	
ATO				_	576	52.60		-9.70	8 7.8		.00	38.44
ATO					576	53.99		-9.60	9 7.28		.00	34.26
ATO					576	55.05		-9.62				37.16
ATO					576	56.384	4	- 9.66			.00	36.38
ATO					576	56.897	7	-8.71			.00	36.98
ATO					576	56.204	1	-7.618		_		38.62
ATO		_			576	58.112		-8.863		_		41.41
		_	AR	G s	576	50.165					. 00	37.48
ATON		_	AR	G 5	76	50.013		9.860			.00	40.55
ATOM			AR	G 5	77	49.156		10.746				43.20
ATOM		6 CA	AR	_	77	47.794		-9.146				41.98
ATOM			AR		77	46.896		-9.372				13.12
ATOM			ARC		77			-8.226		11.		4.21
ATOM	4519	CD	ARC		77	47.206		6.910				5.21
ATOM	4520	) NE	ARC		77	46.402		-5.766	6.941			7.50
ATOM		_	ARG			46.172	-	4.734	7.948			7.58
ATOM				_	77	45.447	-	3.641	7.752			
ATOM	4526				77	44.882	-	3.421	6.574		_	7.63
ATOM	4529			_	77	45.256		2.789	8.747			9.05
ATOM	4530	_	ARG			47.241		0.715	6.821			9.88
ATOM	4531	_	ARG			47.297	-1	1.015	5.627			3.10
ATOM	4533	N	GLN			53.448	-1	3.666	7.976		-	3.86
ATOM	4534	CA	GLN	59	4	52.231		3.872	8.759			4.97
ATOM		CB	GLN	59	4	51.419	-1	5.042		1.0		5.30
	4535	С	GLN	59	4	52.582	~14	4.116	8.200	1.0		7.44
ATOM	4536	0	GLN	59	4	53.162	-14	5.145	10.224	1.0		5.02
ATOM	4537	N	LEU	59	5	52.218	-1:	2.145	10.583	1.0	0 67	1.47
ATOM	4539	CA	LEU	59		52.499	-13	3.151	11.058	1.0		.86
ATOM	4540	CB	LEU	59		52.597	-13	3.187	12.480	1.0		.77
ATOM	4541	CG	LEU	59			-11	751	12.987	1.0		. 35
MOTA	4542	CD1	LEU	599		53.471		.905	12.051	1.00		.70
MOTA	4543	CD2	LEU			53.307		.427	12.322	1.00		.61
ATOM	4544	C		599		54.923		.324	12.175	1.00	_	
ATOM	4545	0	LEU	595		51.482		. 985	13.290	1.00		.38
ATOM	4546		LEU	595		50.302		.026	12.951			. 49
ATOM		N	SER	596		51.969		.647	14.338	1.00	_	. 36
ATOM	4548	CA	SER	596	;	51.134		.447		1.00		
	4549	CB	SER	596		51.905	-16	.669	15.222	1.00		
ATOM	4550	OG	SER	596			-16	. 309	15.721	1.00		13
CCCD :-							_0	. 202	16.698	1.00	54.	98
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MOTA 4552 C SER 596 50.723 -14.597 16.415 1.00 54.73 ATOM 4553 0 1.00 SER 596 51.348 -13.579 16.704 53.29 ATOM 4554 N SER 597 49.704 -15.051 17.137 1.00 55.09 MOTA 4556 CA SER 597 49.215 -14.337 18.307 1.00 56.44 **ATOM** 4557 CB SER 597 48.178 -15.185 19.044 1.00 59.14 MOTA 4558 OG SER 597 47.455 -16.009 1.00 18.138 65.57 MOTA 4560 C SER 597 50.387 -14.026 19.238 1.00 55.64 ATOM 4561 SER 50.430 0 597 -12.966 19.856 1.00 56.04 ATOM 4562 N LYS 598 51.345 -14.948 19.315 1.00 54.91 **ATOM** 4564 CA LYS 598 52.528 -14.773 20.161 1.00 54.25 MOTA 4565 CB LYS 598 53.287 -16.096 20.311 1.00 54.23 ATOM 4566 CG LYS 598 54.236 -16.138 21.494 1.00 55.12 **ATOM** 4567 CD LYS 598 55.009 -17.448 21.523 1.00 59.41 MOTA 4568 CE LYS 598 55.711 -17.679 22.858 1.00 58.10 ATOM 4569 NZ LYS 598 54.750 -17.983 23.959 1.00 56.10 MOTA 4573 С LYS 598 53.439 -13.716 19.536 1.00 52.32 **ATOM** 4574 0 LYS 598 53.986 -12.869 20.249 1.00 52.23 MOTA 4575 N ASP 599 53.573 -13.768 18.208 1.00 47.57 ATOM 4577 CAASP 599 54.389 -12.818 17.466 1.00 45.47 **ATOM** 4578 CB ASP 599 54.324 -13.101 15.959 1.00 49.05 **ATOM** 4579 CGASP 55.245 599 -14.238 15.525 1.00 54.16 **ATOM** 4580 ODI ASP 56.242 599 -14.503 16.223 1.00 61.34 ATOM 4581 OD2 ASP 599 54.992 -14.863 14.471 1.00 55.80 MOTA 4582 C ASP 599 53.933 -11.383 17.721 1.00 43.55 MOTA 4583 0 ASP 599 54.762 -10.491 17.895 1.00 44.34 MOTA 4584 N LEU 600 52.622 -11.160 17.751 1.00 39.73 MOTA 4586 CALEU 600 52.104 -9.82L 17.989 1.00 37.64 ATOM 4587 CB LEU 600 50.597 -9.743 17.719 1.00 35.42 ATOM 4588 CG LEU 600 50.075 ..9.951 16.287 1.00 33.95 MOTA 4589 CD1 LEU 600 48.621 -9.552 16.262 1.00 36.59 ATOM 4590 CD2 LEU 600 50.841 -9.139 15.265 1.00 28.40 ATOM 4591 -9.347 C LEU 600 52.429 19.402 1.00 38.24 **ATOM** 4592 0 LEU 600 52.817 -8.193 19.590 1.00 38.28 **ATOM** 4593 N VAL 601 52.305 -10.235 20.391 1.00 38.77 **ATOM** 4595 CA VAL 601 52.610 -9.855 21.772 1.00 38.87 MOTA 4596 CB VAL 601 52.121 -10.906 22.812 1.00 38.03 **ATOM** 4597 CG1 VAL 601 52.150 -10.303 24.223 1.00 36.21 ATOM 4598 CG2 VAL 601 50.710 -11.332 22.504 1.00 39.07 ATOM 4599 C VAL 601 54.123 -9.662 21.887 1.00 38.98 **ATOM** 4600 601 0 VAL 54.601 -8.757 22.580 1.00 39.93 **ATOM** 4601 N SER 602 54.861 -10.488 21.155 1.00 37.35 MOTA 4603 CA SER 602 56.311 -10.422 21.126 1.00 37.11 MOTA 4604 CB SER 602 56.853 -11.469 20.154 1.00 39.38 **ATOM** 4605 OG SER 602 -11.413 58.265 20.061 1.00 46.76 MOTA 4607 SER C 602 56.695 -9.020 20.664 1.00 35.43 MOTA 4608 0 SER 602 57.493 -8.339 21.315 1.00 35.01 ATOM ' 56.091 4609 N CYS 603 -8.586 19.561 1.00 33.42 MOTA 4611 CA CYS 603 56.329 -7.254 19.015 1.00 32.18 **ATOM** 4612 CB CYS 603 55.449 -7.035 17.790 1.00 32.38 MOTA 4613 SG CYS 603 55.440 -5.365 17.123 0.50 35.11 PRT1 ATOM 4614 C CYS 603 56.074 -6.167 20.059 1.00 31.20 ATOM 4615 0 CYS 603 56.862 -5.234 20.185 1.00 32.44 ATOM 4616 N ALA 604 55.001 -6.321 20.828 1.00 29.74 MOTA

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CA

ALA

604

54.640

-5.363

21.872

1.00

32.26



ATO	OM 46	10 0							
ATO				LA 604 LA 604	53.232			2 1.00	31.75
ATO			AI		55.656				
ATO		-	TY		55.933			1 1.00	
ATO					56.186			5 1.00	
ATC					57. <b>1</b> 76			3 1.00	
ATC					57.447	- •			36.12
ATO					58.562				34.75
ATO					58.415	-8.23			34.30
ATO					59.444	-8.499		1.00	36.26
ATO	M 463				59.773	-9.021			37.39
ATO			TYI		60.812	-9.288		1.00	37.81
ATO			TYI		60.641	-9.027			38.34
ATO			TY		61.662	-9.324		1.00	42.09
ATO		_	TYF		58.475	-5.972			34.98
ATON		_	GLN	_	58.981	-5.171		1.00	35.83
ATOM			GLN		58.996	-6.247		1.00	33.99
ATOM	1 4639		GLN		60.218	-5.620	22.315	1.00	33.60
ATOM		_	GLN		60.506	-6.111	20.894	1.00	31.37
ATOM	1 4643		GLN		60.858	-7.584	20.786	1.00	32.05
ATOM					61.175	-8.015	19.354	1.00	30.33
ATOM	4643				62.145	-7.558	18.754	1.00	30.84
ATOM		C	GLN		60.353 60.123	-8.895	18.810	1.00	33.75
ATOM	4647	0	GLN		61.070	-4.079	22.321	1.00	34.86
ATOM	4648	N	VAL		58.975	-3.390	22.702	1.00	37.54
ATOM		CA	VAL	607	58.748	-3.555	21.904	1.00	32.89
ATOM	4651	CB	VAL	607	57.426	-2.114	21.983	1.00	30.80
ATOM	4652	CG1	VAL	607	57.121	-1.777 -0.299	21.120	1.00	28.82
ATOM	4653	CG2	VAL	607	57.541	~2.204	21.191	1.00	25.36
ATOM	4654	C	VAL	607	58.747	-1.532	19.661	1.00	23.37
ATOM	4655	O	VAL	607	59.359	-0.486	23.312	1 00	30.48
ATOM	4656	N	ALA	608	58.106	-2.225	23.563 24.255		29.42
ATOM	4658	CA	ALA	608	58.064	-1.761	25.646		30.07
ATOM	4659	CB	ALA	608	57.027	-2.548	26.452		30.14
ATOM ATOM	4660	C	ALA	608	59.455	-1.849	26.305		28.49
ATOM	4661	0	ALA	608	59.791	-1.054	27.198		31.25
ATOM	4662 4664	N	ARG	609	60.257	-2.819	25.870		28.90 31.61
ATOM	4665	CA	ARG	609	61.608	-2.979	26.393		31.99
ATOM	4666	CB	ARG	609	62.253	-4.245	25.856		34.93
ATOM	4667	CG	ARG	609	61.606	-5.507	26.317		10.82
ATOM	4668	CD	ARG	609	62.633	-6. <b>6</b> 06	26.397		12.68
ATOM	4670	NE CZ	ARG	609	63.275	-6.621	27.705	_	13.85
MOTA	4671	NH1	ARG	609	64.332	-7.364		<u> </u>	4.73
ATOM	4674	NH2	ARG	609	64.889	-8.162		<b>.</b>	1.40
ATOM	4677	C	ARG	609	64.803	-7.341			4.85
ATOM	4678	0	ARG	609	62.459	-1.796			3.70
ATOM	4679	N	ARG	609	63.130	-1.174			5.94
ATOM	4681	CA	GLY GLY	610	62.459	-1.511	<b>a</b>		1.22
ATOM	4682	C		610	63.232	-0.391	<b>-</b>	_	7.21
ATOM	4683	0	GLY GLY	610	62.819	0.875	24.865		5.81
ATOM	4684	N		610	63.665		25.300		6.21
ATOM	4686	CA	MET	611 611	61.511	1.056			7.12
ATOM	4687			611	60.969		25. <b>69</b> 5 j		8.82
		-		~	59.457	2.288	25.524		9.29

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ATOM	4688	CG	MET	611	59.004	2.706	24.135	1.00	31.07
ATOM	4689	SD	MET	611	59.732	4.286	23.617	1.00	28.38
MOTA	4690	CE	MET	611	59.155	5.431	24.922	1.00	28.34
MOTA	4691	С	MET	611	61.341	2.261	27.178	1.00	30.34
ATOM	4692	0	MET	611	61.596	3.334	27.730	1.00	31.73
ATOM	4693	N	GLU	612	61.347	1.109	27.837	1.00	32.72
MOTA	4695	CA	GLU	612	61.723	1.057	29.253	1.00	35.46
ATOM	4696	CB	GLU	612	61.603	-0.370	29.792	1.00	34.70
MOTA	4697	CG	GLU	612	62.029	-0.516	31.237	1.00	32.31
ATOM	4698	CD	GLU	612	62.135	1.968	31.688	1.00	33.14
MOTA	4699	OE1	GLU	612	62.546	-2.834	30.883	1.00	30.79
ATOM	4700	OE2	GLU	612	61.826	-2.240	32.867	1.00	36.13
MOTA	4701	C	GLU	612	63.178	1.544	29.353	1.00	36.43
ATOM	4702	0	GLU	612	63.534	2.319	30.261	1.00	35.38
ATOM	4703	N	TYR	613	63.999	1.107	28.391	1.00	35.47
ATOM	4705	CA	TYR	613	65.403	1.507	28.334	1.00	33.16
ATOM	4706	CB	TYR	613	66.156	0.743	27.241	1.00	31.33
MOTA	4707	CG	TYR	613	67.612	1.146	27.132	1.00	33.03
MOTA	4708	CD1	TYR	613	68.584	0.544	27.931	1.00	36.69
MOTA	4709	CE1	TYR	613	69.930	0.927	27.851	1.00	36.82
ATOM	4710	CD2	TYR	613	68.021	2.148	26.247	1.00	33.49
ATOM	4711	CE2	TYR	613	69.352	2.540	26.157	1.00	34.73
ATOM	4712	CZ	TYR	613	70.307	1.927	26.963	1.00	37.07
ATOM	4713	OH	TYR	613	71.632	2.318	26.896	1.00	36.77
ATOM	4715	С	TYR	613	65.539	3.005	28.088	1.00	31.82
ATOM	4716	С	TYR	613	66.256	3.682	28.814	1.00	34.75
ATOM	4717	N	LEU	614	64.836	3.536	27.090	1.00	28.44
ATOM	4719	CA	LEU	614	64.931	4.956	26.793	1.00	25.67
ATOM	4720	CB	LEU	614	64.089	5.319	25.569	1.00	24.75
MOTA	4721	CC	LEU	614	64.545	4.778	24.208	1.00	23.73
ATOM	4722	CD1	LEU	614	63.594	5.257	23.125	1.00	20.54
MOTA	4723	CD2	LEU	614	65.983	5.213	23.894	1.00	23,21
MOTA	4724	C	LEU	614	64.499	5.761	28.001	1.00	28.30
MOTA	4725	0	LEU	614	65.110	6.770	28.345	1.00	27.09
ATOM	4726	N	ALA	615	63.470	5.272	28.683	1.00	32.73
ATOM	4728	CA	ALA	615	62.955	5.945	29.871	1.00	34.10
ATOM	4729	СВ	ALA	615	61.625	5.314	30.314	1.00	33.68
ATOM	4730	С	ALA	615	63.986	5.913	31.007	1.00	33.84
ATOM	4731	0	ALA	615	64.112	6.885	31.753	1.00	34.95
MOTA	4732	N	SER	616	64.722	4.809	31.134	1.00	32.69
ATOM	4734	CA	SER	616	65.738	4.703	32.175	1.00	33.50
MOTA	4735	CB	SER	616	66.287	3.277	32.285	1.00	28.27
ATOM	4736	OG	SER	616	67.076	2.935	31.165	1.00	25.54
ATOM	4738	С	SER	616	66.870	5.678	31.865	1.00	35.43
ATOM	4739	0	SER	616	67.637	6.061	32.755	1.00	37.32
ATOM	4740	N	LYS	617	66.971	6.060	30.592	1.00	34.80
MOTA	4742	CA	LYS	617	67.975	7.010	30.143	1.00	33.01
MOTA	4743	СВ	LYS	617	68.508	6.620	28.776	1.00	33.18
ATOM	4744	CG	LYS	617	69.224	5.302	28.797	1.00	35.64
MOTA	4745	CD	LYS	617	70.423	5.380	29.710	1.00	40.31
ATOM	4746	CE	LYS	617	71.075	4.025	29.863	1.00	43.03
MOTA	4747	NZ	LYS	617	72.426	4.152	30.449	1.00	45.54
ATOM	4751	C	LYS	617	67.360	8.397	30.102	1.00	32.87
ATOM	4752	0	LYS	617	67.892	9.308	29.470	1.00	34.06
			-			• •			

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•	ATOM	4753	N	LYS	C 3 6							
i	ATOM	4755	CA		618	66.2		8.542	30.7	772	1 00	
1		4756		LYS	618	65.5	00	9.808			1.00	33.53
		4757	CB	LYS	618	66.3	84	10.842			1.00	33.28
		4758	CG	LYS	618	66.9		10.367	_		1.00	37.22
			CD	LYS	618	65.9			32.8		1.00	43.11
		1759	CE	LYS	618	66.5		0.278	33.9		1.00	49.82
		760	NZ	LYS	618	65.66		9.636	35.1	99	1.00	55.20
		1764	C	LYS	618			9.853	36.4		00	61.31
	TOM 4	765	_	LYS		65.01		0.359	29.5		00	
. A'	TOM 4	766		CYS	618	64.65		1.530	29.4			31.57
A'					619	64.95		9.506	28.52		.00	31.10
				CYS	619	64.51		9.922			.00	31.04
				CYS	619	65.21		9.065	27.19		.00	29.21
				CYS	619	64.78			26.12		.00 .	28.55
	-			YS	619	62.99		9.400	24.39		.00	26.31
			) (	YS	619	62.37		849	27.05		. 00	30.91
			1 1	LE	620			8.827	27.36		00	31.18
					620	62.411		.967	26.63	_		
AT	OM 47	76 c		_		60.981		.073	26.41	_		29.48
AT	OM 47				620	60.402	12	.344	27.06	_		29.34
ATO					620	58.944		. 535	26.649			28.12
ATO			_		620	60.521					00	28.76
ATO					620	60.062			28.581		00	28.36
ATO				E (	520	60.852			29.270			25.55
ATO				Æ (	520	61.254	-		24.908			30.97
	• / (	•••	H	S 6	21	60.307			24.336	1.0		33.88
ATO		4-4	H F	_	21	60.148			24.284	1.0		1.55
ATO		35 CE	з ні		21	50.148		080	22.831	1.0	-	1.85
ATO.		6 CG		_	21	59.721	8.		22.425		_	1.05
ATO		7 CD				59.913	8.		20.979			8.27
ATO!	M 478				21	60.608	7.		0.356			4.68
ATO	M 479			-	21	59.354			9.973	1.0		4.39
ATON			_	_	21	59.691				1.0		5.87
ATOM		_			21	60.444			8.798	1.0		7.65
ATOM	• • • •		HIS		21	59.187	11.0		9.007	1.0		5.80
ATOM	_	_	HIS	62	21	59.387			2.224	1.0		1.38
ATOM			ARC	62	2	58.080	11.5		1.104	1.00	_	1.74
	,,,		ARG				11.3	74 2	2.898	1.00		.17
ATOM		CB	ARG	62		57.093	12.3		2.425	1.00		.27
ATOM		CG	ARG			57.718	13.7	46 22	2.298	1.00		
ATOM			ARG			58.261	14.2		3.601	1.00		.63
ATOM	4801					58.661	15.7		.530			.47
MOTA	4803		ARG	62		59.129	16.1		.842	1.00		. 76
ATOM	4804	-2	ARG	62		60.299	15.82		.375	1.00		.09
ATOM	4807	NH1		62	2	61.132	15.04			1.00		. 86
ATOM		NH2	ARG	622	2	60.606	16.16		.699	1.00	61.	.20
ATOM	4810	C	ARG	622		56.324			.624	1.00	58.	
	4811	0	ARG	622		55.300	11.99		.151	1.00	37.	
ATOM	4812	N	ASP	623		55.300	12.61		.867	1.00	38.	
MOTA	4814	CA	ASP	623		56.805	11.03			1.00		
ATOM	4815	СВ	ASP		•	6.075	10.65			1.00	36.	
ATOM	4816	CG		623	-	6.581	11.40	_			36.	
ATOM	4817		ASP	623	5	5.635	11.24		<b>.</b> .	1.00	39.	
ATOM	4818	OD1	ASP	623		6.077	11.49			1.00	48.	
ATOM		OD2	ASP	623		4.445	10 00			1.00	49.	
	4819	С	ASP	623		6.126	10.87		872	1.00	49.6	
ATOM	4820	0	ASP	623		6.325	9.143		967 j	1.00	33.3	
ATOM	4821	N	LEU	624			8.650			.00	31.7	
MOTA	4823	CA	LEU	624	5	5.999	8.404			.00		
				024	5	6.014	6.954	19.		.00	30.4	
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MOTA	4824	CB	LEU	624	55.983	6.307	21.342	1.00	27.43
MOTA	4825	CG	LEU	624	55.949	4.778	21.441	1.00	28.69
MOTA	4826	CD1	LEU	624	57.139	4.132	20.731	1.00	24.75
MOTA	4827	CD2	LEU	624	55.927	4.389	22.894	1.00	27.39
ATOM	4828	C	LEU	624	54.803	6.532	19.109	1.00	31.22
MOTA	4829	0	LEU	624	53.680	6.952	19.380	1.00	33.44
MOTA	4830	N	ALA	625	55.053	5.763	18.054	1.00	28.85
MOTA	4832	CA	ALA	625	54.009	5.286	17.159	1.00	26.93
ATOM	4833	CB	ALA	625	53.559	6.400	16.227	1.00	25.03
ATOM	4834	С	ALA	625	54.642	4.162	16.356	1.00	28.44
ATOM	4835	0	ALA	625	55.863	4.065	16.317	1.00	31.32
MOTA	4836	N	ALA	626	53.828	3.329	15.705	1.00	29.14
MOTA	4838	CA	ALA	626	54.344	2.205	14.905	1.00	28.42
MOTA	4839	CB	ALA	626	53.192	1.357	14.353	1.00	27.37
MOTA	4840	C	ALA	626	55.231	2.698	13.771	1.00	26.38
MOTA	4841	0	ALA	626	56.195	2.041	13.395	1.00	26.12
ATOM	4842	N	ARG	627	54.890	3.861	13.230	1.00	27.16
ATOM	4844	CA	ARG	627	55.669	4.474	12.158	1.00	28.44
ATOM	4845	CB	ARG	627	55.022	5.794	11.733	1.00	28.19
ATOM	4846	CG	ARG	627	54.889	6.793	12.867	1.00	30.34
ATOM	4847	CD	ARG	627	54.456	8.155	12.361	1.00	34.08
MOTA	4848	NE	ARG	627	54.081	9.024	13.471	1.00	35.58
ATOM	4850	CZ	ARG	627	52.849	9.123	13.950	1.00	35.55
ATOM	4851	NH1	ARG	627	51.860	8.422	13.420	1.00	35.67
ATOM	4854	NH2	ARG	627	52.618	9.898	14.993	1.00	40.81
ATOM	4857	С	ARG	527	57.108	4.733	12.630	1.00	28.06
ATOM	4858	0	ARG	627	58.044	4.737	11.825	1.00	29.80
MOTA	4859	N	ASN	628	57.272	4.935	13.940	1.00	28.50
MOTA	4861	CA	ASN	628	58.582	5.195	14.544	1.00	26.14
ATOM	4862	CB	ASN	628	58.494	6.340	15.551	1.00	23.55
MOTA	4863	CG	ASN	628	58.319	7.681	14.874	1.00	27.48
MOTA	4864	OD1	ASN	628	58.874	7.919	13.800	1.00	34.12
MOTA	4865	ND2	ASN	628	57.543	8.556	15.479	1.00	23.21
ATOM	4868	С	ASN	628	59.263	3.965	15.153	1.00	26.76
MOTA	4869	0	ASN	628	60.202	4.078	15.948	1.00	26.90
MOTA	4870	N	VAL	629	58.774	2.794	14.767	1.00	27.02
MOTA	4872	CA	VAL	629	59.344	1.523	15.186	1.00	27.81
MOTA	4873	CB	VAL	629	58.298	0.622	15.864	1.00	26.83
MOTA	4874	CG1	VAL	629	58.876	-0.766	16.115	1.00	20.74
MOTA	4875	CG2	VAL	629	57.836	1.259	17.165	1.00	22.49
ATOM	4876	С	VAL	629	59.781	0.895	13.861	1 00	28.61
MOTA	4877	0	VAL	629	58.983	0.809	12.924	1.00	28.76
ATOM	4878	N	LEU	630	61.059	0.557	13.746	1.00	30.35
ATOM	4880	CA	LEU	630	61.576	-0.033	12.514	1.00	32.42
ATOM	4881	CB	LEU	630	62.824	0.725	12.040	1.00	32.28
ATOM	4882	CG	LEU	630	62.697	2.249	11.880	1.00	27.75
MOTA	4883	CD1	LEU	630	64.019	2.860	11.469	1.00	24.71
MOTA	4884	CD2	LEU	630	61.611	2.582	10.872	1.00	27.70
MOTA	4885	С	LEU	630	61.895	-1.488	12.799	1.00	32.89
MOTA	4886	0	LEU	630	62.167	-1.838	13.943	1.00	32.32
MOTA	4887	N	VAL	631	61.831	-2.336	11.774	1.00	34.81
MOTA	4889	·CA	VAL	631	62.087	-3.772	11.943	1.00	33.87
ATOM	4890	CB	VAL	631	60.818	-4.616	11.597	1.00	31.60
ATOM	4891	CG1	VAL	631	60.929	-6.004	12.197	1.00	30.84

AT	OM 48	392 (	G2 1	/AL 63					
ΑT		393		/AL 63 /AL 63	· · · <del>-</del>			9 1.00	25.53
AT		194				– –			
AT		95 N	. *				9 9.89		
AT	OM 48		-					0 1.00	_
AT	OM 48	98 C	_		·	- <del>-</del>			00
ATO	OM 48		_	HR 632 HR 632					50
ATO	OM 49	_						3 1.00	
ATO	OM 49	_						1.00	
ATO				HR 632 HR 632					
ATC		_					10.382		41.24
ATC							9.511	_	42.32
ATC					050		8.703	1.00	44.34
ATO					67.314		7.912		46.06
ATO					67.205		6.898	1.00	49.87
ATO.					66.380	_	5.629	-	53.04
ATO					65.637		5.570	1.00	51.31
ATO			GL		66.479	-10.226	4.667	1.00	55.48
ATO			GL		65.708	-9.526	9.600	1.00	44.58
ATO			AS:		64.974	-10.423	9.207	1.00	46.56
ATON			AS		66.201	-9.493	10.833	1.00	44.12
ATON	491		ASI		65.961	-10.583	11.759	1.00	44.23
ATOM	1 4918		ASI		67.221	-10.867	12.580	1.00	50.17
ATOM					68.443	-11.181	11.697	1.00	56.79
ATOM					68.363	-12.113	10.857	1.00	59.62
ATOM	4921		ASF		69.482	-10.490	.11.837	1.00	58.62
ATOM	4922		ASP		64.756	-10.331	12.644	1.00	43.26
MOTA		N	ASN		64.652	-10.879	13.733	1.00	43.58
ATOM		CA	ASN		63.858	-9.475	12.165	1.00	43.97
ATOM	4926		ASN		62.612	-9.126	12.847	1.00	43.66
ATOM	4927		ASN		61.698	-10.355	12.930	1.00	46.94
ATOM	4928	OD1	ASN	_	61.413	-10.958	11.572	1.00	48.19
ATOM	4929	ND2	ASN	635	60.831 61.832	-10.314	10.702	1.00	51.42
ATOM	4932	C	ASN	635	62.694	-12.198	11.380		49.44
ATOM	4933	0	ASN	635	61.774	-8.463	14.216	1.00	43.03
ATOM	4934	N	VAL	636	63.763	-8.596	15.031	1.00	43.03
ATOM	4936	CA	VAL	636	63.915	-7.712	14.467	1.00	42.69
ATOM	4937	CB	VAL	636	65.406	-7.034	15.756	1.00	38.30
ATOM	4938	CG1	VAL	636	65.555	-6.861	16.134	1.00	37.92
ATOM	4939	CG2	VAL	636	66.052	-6.040 -8.226	17.421	1.00	37.14
ATOM	4940	C	VAL	636	63.251				37.55
ATOM	4941	0	VAL	636	63.486				35.75
ATOM	4942	N	MET	637	62.355				36.28
ATOM	4944	CA	MET	637	61.672				34.73
ATOM	4945	CB	MET	637	60.456				33.22
ATOM	4946	CG	MET	637	59.364				4.83
ATOM	4947	SD	MET	637	58.661			1.00 3	4.41
ATOM	4948	CE	MET	637	58.869		15.589	1.00 3	3.19
ATOM	4949	C	MET	637	62.677	<b>^ ~ ~ ~ ~</b>		1.00 2	9.73
ATOM	4950	0	MET	637	63.281				3.75
ATOM	4951	N	LYS	638	62.839			1.00 3	1.79
ATOM	4953	CA	LYS	638	63.774			00 3	1.83
ATOM	4954	CB	LYS	638	64.986			00 2	8.17
ATOM	4955	CG	LYS	638	66.006				4.98
CCCP :-					50.000	-1.967 1	6.400 1	.00 2	3.17
SSSD/55	145 VA1								

ATOM	4956	CD	LYS	638	67.193	-1.916	15.470	1.00	25.04
ATOM	4957	CE	LYS	638	68.212	-2.969	15.847	1.00	24.79
ATOM	49,58	NZ	LYS	638	68.747	-2.765	17.220	1.00	24.91
ATOM	4962	C	LYS	638	63.165	0.445	16.986	1.00	26.04
MOTA	4963	0	LYS	638	62.803	0.958	15.936	1.00	24.44
ATOM	4964	N	ILE	639	63.052	1.031	18.181	1.00	25.14
ATOM	4966	CA	ILE	639	62.508	2.376	18.351	1.00	25.68
ATOM	4967	CB	ILE	639	62.589	2.863	19.839	1.00	27.40
MOTA	4968	CG2	ILE	639	61.875	4.189	19.984	1.00	18.94
MOTA	4969	CG1	ILE	639	62.019	1.827	20.826	1.00	26.05
ATOM	4970	CD1	ILE	639	60.517	1.667	20.792	1.00	25.07
ATOM	4971	С	ILE	639	63.387	3.338	17.543	1.00	25.82
ATOM	4972	0	ILE	639	64.619	3.283	17.642	1.00	25.76
ATOM	4973	N	ALA	640	62.758	4.231	16.783	1.00	25.92
MOTA	4975	CA	. ALA	640	63.477	5.218	15.976	1.00	26.12
MOTA	4976	CB	ALA	640	63.222	4.964	14.506	1.00	26.54
MOTA	4977	C	ALA	640	63.042	6.643	16.344	1.00	26.33
ATOM	4978	0	ALA	640	61.996	6.828	16.974	1.00	26.20
MOTA	4979	И	ASP	641	63.863	7.637	15.993	1.00	26.59
ATOM	4981	CA	ASP	641	63.545	9.052	16.245	1.00	28.09
ATOM	4982	CB	ASP	641	62.217	9.443	15.593	1.00	31.43
ATOM	4983	CG	ASP	641	62.346	9.762	14.107	1.00	36.81
ATOM	4984	OD1	ASP	641	63.409	9.478	13.500	1.00	40.24
ATOM	4985	OD2	ASP	641	61.356	10.299	13.548	1.00	40.49
MOTA	4986	C	ASP	641	63.455	9.442	17.700	1.00	28.40
ATOM	4987	O	ASP	641	62.825	10.446	18.041	1.00	29.30
MOTA	4988	N	PHE	642	64.080	8.658	18.564	1.00	30.27
ATOM	4990	CA	PHE	642	64.044	8.943	19.992	1.00	30.97
ATOM	4991	CB	PHE	642	64.327	7.664	20.787	1.00	24.64
ATOM	4992	CG	PHE	642	65.673	7.063	20.505	1.00	20.96
MOTA	4993	CD1	PHE	642	66.812	7.539	21.163	1.00	16.89
ATOM	4994	CD2	PHE	642	65.806	6.026	19.576	1.00	16.23
ATOM	4995	CE1	PHE	642	68.372	6.990	20.900	1.00	18.35
ATOM	4996	CE2	PHE	642	67.051	5.471	19.305	1.00	18.76
ATOM	4997	CZ	PHE	642	68.195	5.954	19.970	1.00	17.91
ATOM	4998	C	PHE	642	65.024	10.045	20.414	1.00	34.53
MOTA	4999	O	PHE	642	64.990	10.503	21.563	1.00	35.23
MOTA	5000	N	GLY	643	65.910	10.433	19.500	1.00	36.40
ATOM	5002	CA	GLY	643	66.888	11.455	19.799	1.00	38.28
ATOM ATOM	5003 5004	C	GLY	643	66.634	12.768	19.093	1.00	41.44
		0	GLY	643	67.482	13.652	19.132	1.00	44.10
ATOM ATOM	5005	N	LEU	644	65.461	12.921	18.484	1.00	45.44
ATOM	5007	CA	LEU	644	65.131	14.144	17.748	1.00	49.14
	5008	CB	LEU	644	63.832	13.975	16.969	1.00	46.26
ATOM	5009	CG	LEU	644	63.823	12.967	15.836	1.00	42.90
MOTA	5010	CD1	LEU	644	62.527	13.134	15.070	1.00	42.68
ATOM	5011	CD2	LEU	644	65.004	13.228	14.934	1.00	45.15
ATOM	5012	C	LEU	644	65.027	15.396	18.605	1.00	53.90
ATOM	5013	0	LEU	644	64.488	15.356	19.715	1.00	56.54
ATOM	5014	N	ALA	645	65.534	16.505	18.068	1.00	57.59
ATOM	5016	CA	ALA	645	65.505	17.794	18.759	1.00	60.15
ATOM	5017	CB	ALA	645	66.539	18.741	18.156	1.00	59.55
ATOM	5018	С	ALA	645	64.112	18.407	18.667	1.00	61.90
ATOM	5019	0	ALA	645	63.393	18.500	19.663	1.00	63.83

	MO	50	20	N	ASP	652	52.09	20 22 -			
AT	MO	50	22	_	ASP	652	-2.02				00 89.91
ΑT	MO'	50	23	_	ASP	652				07 1.0	0 89.75
AT	OM	502			ASP	652				37 1.0	
AT	OM	502			ASP		20.10			07 1.0	
AT	OM	502		_	ASP	652	49.02		96 12.09		005
ATO	OM	502		_ `		652	50.25		22 10.43		
ATO		502			SP	652	50.14		0 14.15		
ATO		502	-	-	SP	652	50.43		9 13.48		
ATO		503		_	YR	653	49.14	5 20.90			
ATC					YR	653	48.318	3 19.73			· <del>-</del>
ATC		503	_		YR	653	47.272				
		503	_		YR	653	47.804				
ATO		503	_		YR	653	47.017				
ATO		503		E1 T	YR	653	47.477		_		
ATO		503		D2 T	YR	653	49.083			-	
ATO		503		E2 T	ľR	653	49.558				93.46
ATO		5038	3 C	Z T	/R	653	48.748				
ATO		5039	OF			653					95.26
ATO		5041	C	TY		653	49.220			9 1.00	
ATO	M !	5042	. 0	TY		653	47.602	19.231		1.00	
ATON	vj g	5043		TY			47.045	18.131			91.33
ATOM		045				654	47.632	20.031	12.962		39.21
ATOM		046				654	46.954	19.673	11.727		
ATOM		047				654	46.205	20.893	11.198		89.09
ATOM		048	CD			654	45.275	. 21.499	12.209		88.23
ATOM		049				654	45.776	22.140			87.65
ATOM		050	CE			654	44.929	22.655	14.312		86.76
ATOM	_	051	CD.			654	43.895	21.396	12.067		87.17
АТОМ	_		CE:			554	43.032	21.912	13.033		88.61
ATOM		052	CZ	TY		554	43.557	22.538	14.153		89.32
ATOM	_	053	OH	TY		554	42.710	23.034		1.00	88.66
		055	G	TYF	₹ €	54	47.857	19.080	15.117	1.00	89.35
ATOM		056	0	TYR	6	54	47.396	18.772	10.651	1.00	29.49
ATOM		057	N	LYS	6	55	49.139		9.552	1.00	88.37
ATOM	50	)59	CA	LYS	6	55	50.056	18.919	10.959	1.00	90.80
ATOM	50	060	CB	LYS		55	51.508	18.356	9.982	1.00	93.18
ATOM	50	61	CG	LYS		55		18.713	10.311	1.00	95.66
ATOM	50	62	CD	LYS		55	52.504	18.133	9.315	1.00	99.82
ATOM	50	63	CE	LYS		55	53.932	18.585	9.562	1.0010	3.58
ATOM	50	64	NZ	LYS		55	54.898	17.833	8.637	1.0010	
ATOM	50	68	C	LYS		55	56.325	18.246	8.821	1.0010	
ATOM	50		ō	LYS			49.884	16.847	9.935	1.00	93.56
ATOM	50		N	LYS		55	49.904	16.182	10.972	1.00	93.72
ATOM	50		CA			56	49.670	16.320	8.735	1.00	94.19
ATOM	50			LYS		66	49.500	14.886	8.545	1.00	
ATOM	50		CB	LYS	65		48.628	14.620	7.320		94.84
ATOM			CG	LYS	65	66	47.155	14.874	7.542	_	94.64
	50		CD	LYS	65	6	46.402	14.709			95.54
ATOM	50		CE	LYS	65	6	44.926	14.449	6.241	1.00	99.56
ATOM	507		NZ	LYS	65	6	44.202	14.327	6.473	1.0010	
ATOM	508		C	LYS	65		50.859		5.173	1.0010	3.77
MOTA	508		0	LYS	65		51.823	14.225	8.368		95.18
ATOM	508	3	N	GLY	66		48.651	14.878	7.956		95.74
ATOM	508	5	CA	GLY	66			9.665	5.782		58.76
ATOM	508		C	GLY	66		47.932	10.910	6.012		56.04
ATOM	508		o	GLY			47.241	10.937	7.364	`	33.90
	_		-	OLI	66	U	46.183	11.552			53.92
SSSD/551	145	ν <b>Ω</b> 1									

ATOM	5088	N	ARG	661	47.838	10.243	8.328	1.00	51.87
ATOM	5090	CA	ARG	661	47.297	10.177	9.679	1.00	48.23
MOTA	5091	CB	ARG	661	47.755	8.891	10.377	1.00	49.74
ATOM	5092	CG	ARG	661	47.506	7.620	9.566	1.00	47.59
ATOM	5093	CD	ARG	661	47.561	6.390	10.446	1.00	51.85
ATOM	5094	NE	ARG	661	47.584	5.155	9.663	1.00	52.94
ATOM	5096	CZ	ARG	661	48.035	3.988	10.117	1.00	52.19
ATOM	5097	NHl	ARG	661	48.503	3.884	11.356	1.00	52.10
ATOM	5100	NH2	ARG	661	48.036	2.926	9.327	1.00	54.43
MOTA	5103.	С	ARG	661	47.722	11.401	10.483	1.00	43.67
ATOM	5104	0	ARG	661	48.658	12.103	10.104	1.00	41.45
ATOM	5105	N	LEU	662	47.019	11.656	11.579	1.00	40.27
ATOM	5107	CA	LEU	662	47.310	12.799	12.437	1.00	37.15
ATOM	5108	CB	LEU	662	46.021	13.533	12.783	1.00	37.39
MOTA	5109	CG	LEU	662	45.301	14.149	11.588	1.00	37.67
MOTA	5110	CD1	LEU	662	43.852	14.428	11.937	1.00	35.38
ATOM	5111	CD2	LEU	662	46.041	15.407	11.163	1.00	39.79
ATOM	5112	С	LEU	662	47.973	12.330	13.716	1.00	34.68
MOTA	5113	0	LEU	662	47.327	11.718	14.568	1.00	33.33
ATOM	5114	N	PRO	663	49.260	12.655	13.892	100	34.11
ATOM	5115	CD	PRO	663	50.086	13.389	12.924	1.00	33.67
ATOM	5116	CA	PRO	663	50:052	12.281	15.068	1.00	33.55
MOTA	5117	СВ	PRO	663	51.367	13.003	14.833	1.00	32.99
ATOM	5118	CG	PRO	663	51.479	12.966	13.328	1.00	36.09
MOTA.	5119	С	PRO	663	49.412	12.665	16.399	1.00	33.55
ATOM	5120	0	PRO	663	49.683	12.036	17.426	1.00	34.11
ATOM	5121	N	VAL	664	48.566	13.697	16.387	1.00	32.63
ATOM	5123	CA	VAL	664	47.874	14.092	17.613	1.00	32.24
ATOM.	5124	CB	VAL	664	46.953	15.327	17.396	1.60	33.24
ATOM	5125	CG1	VAL	664	47.779	16.583	17.252	1.00	35.01
ATOM	5126	CG2	VAL	664	46.089	15.154	16.155	1.00	35.44
MOTA	5127	C	VAL	664	47.072	12.896	18.150	1.00	31.08
MOTA	5128	0	VAL	664	46.866	12.760	19.360	1.00	31.49
ATOM	5129	N	LYS	665	46.710	11.978	17.255	1.00	29.75
ATOM	5131	CA	LYS	665	45.956	10.788	17.638	1.00	28.83
MOTA	.5132	CB	LYS	665	45.411	20.083	16.397	1.00	29.52
MOTA	- 5133	CG	LYS	665	44.242	10.835	15.797	1.00	27.21
ATOM	5134	CD	LYS	665	43.905	10.431	14.397	1.00	27.25
ATOM	5135	CE	LYS	665	42.684	11.228	13.931	1.00	28.63
ATOM	5136	NZ	LYS	665	42.266	10.902	12.545	1.00	25.33
ATOM	5140	С	LYS	665	46.718	9.830	18.537	1.00	29.03
MOTA	5141	0	LYS	665	46.152	8.869	19.046	1.00	28.37
ATOM	5142	N	TRP	666	47.994	10.123	18.765	1.00	30.40
ATOM	5144	CA	TRP	666	48.825	9.296	19.628	1.00	31.10
ATOM	5145	CB	TRP	666	50.123	8.906	18.917	1.00	29.53
MOTA	5146	CG	TRP	666	49.946	7.781	17.966	1.00	27.03
MOTA	5147	CD2	TRP	666	49.407	7.853	16.638	1.00	25.06
MOTA	5148	CE2	TRP	666	49.418	6.546	16.116	1.00	23.83
ATOM	5149	CE3	TRP	666	48.924	8.899	15.835	1.00	26.08
MOTA	5150	CD1	TRP	666	50.257	6.475	18.186	1.00	20.75
MOTA	5151	NE1	TRP	666	49.937	5.729	17.086	1.00	24.92
ATOM	5153	CZ2	TRP	666	48.962	6.245	14.832	1.00	23.95
MOTA	5154	CZ3	TRP	666	48.466	8.604	14.548	1.00	29.09
ATOM	5155	CH2	TRP	666	48.491	7.282	14.060	1.00	29.22

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	ATOM	5156	C	TOD							
	ATOM	5157	ō	TRP	666	49.	174	10.049	20 000		
	ATOM	5158	N	TRP	666	49.	701	•	20.896	1.00	33.20
	ATOM	5160		MET	667	48.			21.849	1.00	34.39
	ATOM	5161	CA	MET	667	49.			20.910		34.82
	ATOM		CB	MET	667	49.	_	12.175	22.056	_	36.31
	ATOM	5162	CG	MET	667	50.		13.645	21.651		10.08
	ATOM	5163	SD	MET	667	50.	_	14.047	20.931	_	
		5164	CE	MET	667	50.	_	15.818 2	0.713	_	2.41
		5165	С	MET	667	50.9		5.928 1	8.949		1.31
	ATOM	5166	0	MET	667	48.2	99 1				5.44
		5167	N	ALA		47.0	81 1		2 20-		7.81
		5169	CA		668	48.9	58 1		_	1.00 3	8.91
	ATOM !	5170	CB		668	48.2	86 1				6.47
Į	ATOM 5	5171	C		668	49.3	08 1:		5.718	1.00 3	7.06
A		172	ō		668	47.5	48 1			1.00 35	5.76
A	_		N		668	48.00			893 1		1.76
			~~		569	46.41		•	.414 1	L.00 38	.04
	_		~ -		669	45.81	_		.608 l		.60
	ma	. ~ -	~~		69	45.61			.282 1	_	.64
	TIO	<b>.</b>		PRO 6	69	44.47			.841 <sub>1</sub>		.25
				PRO 6	69	44.38		.827 <sub>27</sub>			. 08
		L78 (	- I	PRO 6	69	46.39	_	.368 27	300		.08
		79 ر	) <u>F</u>		69	46.39		486 27	E 2 6	- • •	04
		.80 N	,		70	46.304	- •	644 27.	_		68
					70	47.13	15.				
AT		83 G	_	LU 67		47.905	16.	_		00 44.	
AT		84 C	_	LU 67		48.596	15.	637 30.		00 45.	
AT		85 C				49.858	14	819 30.	_	00 46.	
AT(						49.588	13	345 30.	n	• •	
ATO	OM 518	-				50.512	12.				35
ATC	DM 518	88 C				48.458	12.9				9
ATC	M 518		GI			48,942	16.8				'O
ATO	M 519		GL	' '		49.174	18.0			00 45.6	
ATO			AL		L	49.546				0 44.7	
ATO		_			l .	50.555	15.9		82 1.0	0 46.1	
ATO			AL		•	51.218	16.4	-		0 46.4	
ATON		_	AL	A 671		49.931	15.2		60 1.0		
ATON			AL			50.485	17.3		33 1.0		
ATOM	4230		LE	J 672	- 2	18.748	18.3		50 1.00		,
ATOM			LEU	672		8.010	16.92	28 25.01	8 1.00		
ATOM			LEU		•	6.010	17.65	57 23.99	0 1.00		
			LEU	_	. 7	6.996	16.70	05 23.34	6 1.00		
ATOM			LEU	_	4	6.202	17.11	3 22.10	5 1.00		
MOTA		CD2	LEU		4	7.114	17.42	5 20.93	2 1.00		
ATOM		С	LEU	672	4	5.269	15.97	7 21.75	_	•	
ATOM	5204	0	LEU		4	7.315	18.92	5 24.51		00.52	
ATOM	5205	N	PHE		4	7.289	19.95	B 23.83	_	55.91	
ATOM	5207	CA	PHE	673	46	5.782	18.846		_	55.72	
ATOM	5208			673	46	6.089	19.977		_	57.88	
ATOM	5209		PHE	673	44	.873	19.484			60.07	
ATOM	5210	CG	PHE	673	43	. 876	70 740			57.08	
ATOM		CD1	PHE	673	43	. 191	18.742		1.00	56.39	
ATOM	5211	CD2	PHE	673	43	. 633	17.653		1.00	57.67	
ATOM	5212	CE1	PHE	673	42	. 281	19.116		1.00		
	5213	CE2	PHE	673	42	. 201	16.939	26.036	1.00	55.36	
ATOM	5214	CZ	PHE	673	4.2	. 724	18.410	24.183	1.00	57.42	
ATOM	5215	C	PHE	673		. 049	17.317	24.720	1.00	55.91	
			- <del></del>	J / J	46.	974	20.854	27.238		56.42	
SSSD/55	145. v01								1.00	63.00	

ATO	M 5216	0	PHE	<b>67</b> 3	46.926	22.085	27.155	1.00	65.31
ATO	M 5217	N	ASP	674	47.786	20.223	28.081	1.00	64.08
ATO	M 5219	CA	ASP	674	48.656	20.954	28.999	1.00	64.97
ATO	M 5220	CB	ASP	674	48.545	20.375	30.409	1.00	<b>65.1</b> 3
ATO	M 5221	CG	ASP	674	47.128	20.358	30.923	1.00	67.33
ATO	M 5222	OD1	ASP	674	46.684	19.283	31.372	1.00	66.68
ATO	M 5223	OD2	ASP	674	46.462	21.416	30.869	1.00	69.20
ATO	M 5224	C	ASP	674	50.132	20.971	28.603	1.00	66.38
ATO	M 5225	0	ASP	674	50.984	21.304	29.434	1.00	68.44
ATO	M 5226	N	ARG	675	50.441	20.585	27.365	1.00	65.68
ATO	M 5228	CA	ARG	675	51.829	20.550	26.883	1.00	63.71
ATO	M 5229	CB	ARG	675	52.321	21.970	26.576	1.00	63.67
OTA	M 5230	CG	ARG	675	51.491	22.685	25.531	1.00	67.65
ATO	M 5231	CD	ARG	675	52.094	24.034	25.146	1.00	73.20
OTA	M 5232	NE	ARG	675	53.382	23.911	24.457	1.00	74.09
OTA	M 5234	CZ	ARG	675	54.159	24.939	24.122	1.00	73.41
ATO	M 5235	NHl	ARG	675	53.788	26.182	24.408	1.00	72.90
OTA	M 5238	NH2	ARG	675	55.324	24.720	23.524	1.00	71.96
ATON	M 5241	С	ARG	675	52.780	19.864	27.876	1.00	61.41
ATO		0	ARG	675	53.960	20.208	27.966	1.00	62.62
ATON	M 5243	N	ILE	676	52.248	18.903	28.627	1.00	59.15
ATO		CA	ILE	676	53.016	18.162	29.623	1.00	56.88
OTA		CB	ILE	676	52.175	17.904	30.891	1.00	56.26
ATON	M 5247	CG2	ILE	675	52.871	16.904	31.807	1.00	53.11
MOTA		CG1	ILE	676	51.920	19.224	31.614	1.00	57.86
MOTA	1 5249	CD1	ILE	676	51.038	19.096	32.835	1.00	61.05
ATON		C	ILE	676	53.494	16.828	29.070	1.00	56.58
ATON		0	ILE	676	52.727	15.869	28.985	1.00	58.12
MOTA		N	TYR	677	54.760	16.773	28.680	1.00	54.34
ATON		CA	TYR	677	55.340	15.556	28.143	1.00	51.14
ATON		CB	TYR	677	56.240	15.868	26.954	1.00	52.37
ATON		CG	TYR	677	55.488	16.315	25.719	1.00	56.21
MOTA		CD1	TYR	677	55.187	17.660	25.512	1.00	56.78
ATOM		CE1	TYR	677	54.534	18.086	24.353	1.00	57.54
ATOM		CD2	TYR	677	55.113	15.395	24.738	1.00	57.82
ATOM		CE2	TYR	677	54.458	15.809	23.571	1.00	59.32
ATOM		CZ	TYR	677	54.177	17.159	23.385	1.00	59.59
ATOM		ОН	TYR	677	53.557	17.589	22.230	1.00	60.15
MOTA MOTA		C	TYR	677	56.124	14.854	29.224	1.00	48.64
ATOM		O M	TYR	677	57.040	15.430	29.812	1.00	50.45
ATOM		N CA	THR THR	678	55.733	13.621	29.510	1.00	44.59
ATOM		CB	THR	678	56.397	12.834	30.524	1.00	42.21
ATOM				678	55.524	12.726	31.791	1.00	43.55
ATOM		OG1 CG2	THR THR	678	54.302	12.045	31.475	1.00	47.42
ATOM		C	THR	678 678	55.190 56.634	14.105	32.327	1.00	48.74
ATOM		0			56.634	11.432	29.992	1.00	39.94
ATOM		N	THR	678 679	56.207	11.085	28.892	1.00	39.34
ATOM			HIS	679	57.312	10.616	30.784	1.00	38.54
ATOM		CA CB	HIS	679 679	57.532	9.248	30.390	1.00	38.29
ATOM		CG	HIS HIS	679 679	58.441	8.546	31.391	1.00	39.51
ATOM				679	59.869	8.997	31.331	1.00	43.13
		CD2	HIS	679	60.630	9.668	32.233	1.00	43.49
ATOM ATOM		ND1	HIS	679	60.694	8.726	30.263	1.00	43.00
AIUM	5283	CE1	HIS	679	61.903	9.201	30.510	1.00	43.62

A	TOM	5284	NE2	HIS	650						
A		5286	C	HIS	679	٠		778 31	.695	1.00	11 60
A	TOM 5	5287	0	HIS	679	-0.19			.359	1.00	0 0
		288		GLN	679	95.05			.593	1.00	
		290	~-	GLN	680				142	1.00	40.00
. A'	TOM 5	291		GLN	680	53.86			209	1.00	38.96
A:	FOM 5	_	<b></b>	GLN	680	53.21		010 32.	543	1.00	38.84
A				GLN	680	53.83			732	1.00	40.90
AT	TOM 5:			3LN	680	53.67			660	1.00	44.42
ÞΤ	OM 5:	~ ~ ~		3LN	680	52.59			908	1.00	44.47
AT		_	`	LN	680	54.767	6.0			1.00	45.52
AT					680	53.013	9.0			1.00	42.06
AT	_	100 N	_ `	LN	680	51.968	8.5			1.00	38.25
AT				ER	681	53.427	10.1				39.27
ATO		_	_	ER	681	52.665	10.5	71 28.1		1.00	37.00
ATO		_		ER	681	52.929	12.0			1.00	38.02
ATO		_		ER	681	54.307	12.28			1.00	40.29
ATO		_	~		681	53.066	9.62			1.00	47.29
ATO		_	٠.		681	52.289	9.36			1.00	37.43
ATC				_	682	54.281	9.07			1.00	37.86
ATO			_		682	54.800	8.10			1.00	35.23
ATO					682	56284	7.82		<b>-</b> .	1.00	33.24
ATO					582	57.224	8.73				31.85
ATO				_	582	58.445	8.53				34.18
ATO					82	56.763	9.62				31.79
ATO		_	AS		82	54.015	6.81				29.15
ATOM		_	AS		82	53.788	ő.08°				31.52
ATON			VA		83	53.653	6.499				31 93
ATOM					83	52.879	5.293				33.14
ATOM					83	52.725	5.095				32.79
ATOM				_	83	51.653	4.059				14.56
ATOM			VAI VAI	_	83	54.050	4.649				2.39
ATOM					B3	51.506	5.338				8.08
ATOM			VAI TRF		93	51.008	4.311				1.45
ATOM	5327		TRP			50.919	6.531	27.14			0.37
ATOM	5328					49.638	6.686	26.464			1.04
ATOM	5329		TRP			49.158	8.137	26.525			1.23
ATOM	5330		TRP			47.913	8.423	25.694			4.14
ATOM	5331	CE2		68		46.573	8.593	26.187			7.17
ATOM	5332	CE3		68		45.755	8.888	25.064			3.61
MOTA	5333	CD1	TRP TRP	68		45.978	8.528	27.452		_	7.91
ATOM	5334	NE1	TRP	68		47.850	8.612	24.337			7.63
ATOM	5336	CZ2	TRP	68		46.560	8.894	23.956			.39
ATOM	5337	CZ3		68		44.380	9.118	25.181	1.0		.76
ATOM	5338	CH2	TRP	684		44.611	8.759	27.563	1.0		. 79
ATOM	5339	C	TRP	684		43.830	9.048	26.428			.53
ATOM	5340	0	TRP	684		49.876	6.294	25.013	1.0	_	.59
ATOM	5341	N	TRP	684		49.254	5.356	24.503	1.0		.99
ATOM	5343		SER	685		50.815	6.992	24.380	1.0		. 82
ATOM	5344	CA	SER	685		51.174	6.738	22.986	1.0		
ATOM	5345	CB	SER	685	ľ	52.444	7.504	22.631	1.0		
ATOM	5345	OG C	SER	685		52.355	8.874	22.986	1.0		
ATOM	5348	C	SER	685		51.3 <b>9</b> 9	5.249	22.737	1.00		
ATOM	5349	O N	SER	685	5	50.968	4.709	21.713	1.00		
	2243	N	PHE	686		52.065	4.582	23.676	1.00		
SSSD/55	145. v01						- ~	0/6	1.00	26.	47

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MOTA	5351	CA	PHE	686	52.325	3.151	23.563	1.00	26.35
ATOM	5352	CB	PHE	686	53.167	2.668	24.754	1.00	25.01
MOTA	5353	CG	PHE	686	53.447	1.182	24.742	1.00	27.24
MOTA	5354	CD1	PHE	686	54.187	0.600	23.712	1.00	24.88
MOTA	5355	CD2	PHE	686	52.915	0.351	25.729	1.00	24.99
MOTA	5356	CE1	PHE	686	54.389	-0.783	23.655	1.00	22.77
ATOM	5357	CE2	PHE	686	53.113	-1.036	25.679	1.00	28.39
ATOM	5358	CZ	PHE	686	53.853	-1.601	24.631	1.00	22.71
ATOM	5359	С	PHE	686	50.997	2.366	23.466	1.00	28.82
ATOM	5360	0	PHE	686	50.892	1.398	22.696	1.00	26.41
ATOM	5361	N	GLY	687	49.988	2.797	24.229	1.00	29.65
ATOM	5363	CA	GLY	687	48.692	2.134	24.194	1.00	29.88
ATOM	5364	С	GLY	687	48.099	2.158	22.794	1.00	29.57
ATOM	5365	o	GLY	687	47.560	1.165	22.300	1.00	30.38
ATOM.	5366	N	VAL	688	48.222	3.310	22.147	1.00	29.19
ATOM	5368	CA	VAL	688	47.718	3.478	20.795	1.00	25.09
ATOM	5369	CB	VAL	688	47.747	4.956	20.359	1.00	22.52
ATOM	5370	CG1	VAL	688	47.106	5.115	18.985	1.00	21.13
ATOM	5371	CG2	VAL	688	47.001	5.810	21.366	1.00	22.50
ATOM	5372	C	VAL	688	48.574	2.636	19.865	1.00	23.82
ATOM	5373	0	VAL	688	48.080	2.132	18.871	1.00	25.39
ATOM	5374	И	LEU	689	49.849	2.463	20.208	1.00	24.46
ATOM	5376	CA	LEU	689	50.764	1.655	19.401	1.00	25.68
ATOM	5377	CB	LEU	689	52.222	1.893	19.834	1.00	25.93
ATOM	5379	CG	LEU	689	53.374	1.307	19.004	1.00	25.01
ATOM	5379	CD1	LEU	689	54.655	2.080	19.257	1.00	25.86
ATOM	5380	CD2	LEU	689	53.593	-0.145	19.318	1.00	24.90
ATOM	5381	C	LEU	689	50.374	0.171	19.531	1.00	26.50
ATOM	5382	Ó	LEU	689	50.464	-0.578	18.558	1.00	27.13
ATOM	5383	N	LEU	690	49.927	-0.234	20.724	1.00	27.76
ATOM	5385	CA	LEU	690	49.481	-1.610	20.980	1.00	28.59
ATOM	5386	СВ	LEU	690	49.087	-1.800	22.447	1.00	30.38
ATOM	5387	CG	LEU	690	50.121	-2.065	23.545	1.00	29.57
ATOM	5388	CD1	LEU	690	49.435	-1.966	24.907	1.00	27.40
ATOM	5389	CD2	LEU	690	50.744	-3.431	23.360	1.00	28.79
ATOM	5390	С	LEU	690	48.242	-1.849	20.134	1.00	28.77
MOTA	5391	0	LEU	690	48.055	-2.922	19.573	1.00	28.07
ATOM	5392	N	TRP	691	47.383	-0.838	20.075	1.00	29.58
ATOM	5394	CA	TRP	691	46.166	-0.921	19.275	1.00	30.53
ATOM	5395	CB	TRP	691	45.327	0.349	19.451	1.00	28.28
ATOM	5396	CG	TRP	691	43.985	0.300	18.769	1.00	25.86
ATOM	5397	CD2	TRP	691	43.702	0.689	17.421	1.00	23.99
ATOM	5398	CE2	TRP	691	42.321	0.498	17.215	1.00	25.08
ATOM	5399	CE3	TRP	691	44.487	1.165	16.367	1.00	20.88
ATOM	5400	CD1	TRP	691	42.791	-0.090	19.314	1.00	23.72
MOTA	5401	NE1	TRP	691	41.786	0.031	18.389	1.00	26.15
ATOM	5403	CZ2	TRP	691	41.704	0.788	15.997	1.00	25.07
ATOM	5404	CZ3	TRP	691	43.883	1.448	15.163	1.00	22.80
ATOM	5405	CH2	TRP	691	42.501	1.251	14.982	1.00	24.95
ATOM	5406	C	TRP	691	46.566	-1.116	17.811	1.00	30.63
ATOM	5407	0	TRP	691	45.943	-1.892	17.093	1.00	33.02
ATOM	5408	N	GLU	692	47.625	-0.431	17.386	1.00	31.00
ATOM	5410	CA	GLU	692	48.130	-0.545	16.018	1.00	29.00
ATOM	5411	CB	GLU	692	49.285	0.426	15.778	1.00	26.55
						0.420	23.770	1.00	20.55

AT	OM 543	12 00							
ATO		_			48.873		6 15.65	1 1.00	29.90
ATO					50.040				
ATO					50.770	3.17			
ATO					50.227				
ATC			GL		48.622	-1.95			
			GL	U 692	48.474	-2.46			02
ATC			IL	E 693	49.258	-2.57			– –
ATO			IL	E 693	49.766	-3.93			=
ATO			IL	€ 693	50.634	-4.360			
ATO	- <del>-</del>	2 CG2	: IL	E 693	51.006	-5.845			0
ATO		3 CG1	ILE		51.909	-3.506		-	
ATO		4 CD1	ILE	693	52.696	-3.693	_	_	30.30
ATO		5 C	ILE		48.638				25.66
ATO		5 0	ILE		48.633	-4.939	· ·	1.00	30.63
ATO	M 5427	7 N	PHE		47.644	-5.738		1.00	31.10
ATO	4 5429	CA	PHE		46.543	-4.858		1.00	32.60
ATOM	4 5430	CB	PHE			-5.793		1.00	33.86
ATON	4 5431		PHE	· - <del>-</del>	45.938	-5.970		1.00	35.66
ATOM	1 5432		PHE		46.941	-6.499	19.559	1.00	35.70
ATOM	1 5433		PHE	694	47.460	-5.684	20.556	1.00	37.18
ATOM	5434		PHE	694	47.449	-7.794	19.426	1.00	34.37
ATOM			PHE	694	48.473	-6.150	21.392	1.00	36.90
ATOM		CZ	PHE	694	48.456	-8.265	20.255	1.00	31.89
ATOM			PHE		48.970	-7.446	21.234	1.00	34.95
ATOM		o	PHE	694	45.532	-5.576	16.049	1.00	34.26
ATOM		N		694	44.702	-6.442	15.787	1.00	37.52
ATOM		CA	THR	695	45.636	-4.441	15.359	1.00	32.23
ATOM		CB	THR	695	44.775	-4.160	14.215	1.00	28.08
ATOM		OG1	THR	695	44.186	-2.728	14.241	1.00	25.71
ATOM	5445	CG2	THR	695	45.237	-1.762	14.228	1.00	24.94
ATOM	5446	C	THR	695	43.353	-2.528	15.468	1.00	23.07
ATOM	5447	0	THR	695	45.615	-4.348	12.955	1.00	27.53
ATOM	5448		THR	695	45.166	-4.066	11.845	1.00	30.89
ATOM	5450	N Gr	LEU	696	46.833	-4.848	13.145	1.00	27.73
ATOM	5451	CA	LEU	696	47.781	-5.081	12.061	1.00	28.99
ATOM		CB	LEU	696	47.370	-6.297	11.226	1.00	27.78
ATOM	5452 5453	CG	LEU	696	47.379	-7.591	12.047	1.00	29.89
ATOM		CD1	LEU	696	4.7.251	-8.823	11.164	1.00	29.96
ATOM	5454	CD2	LEU	696	48.668	-7.656	12.803	1.00	30.20
ATOM	5455 5456	C	LEU	696	48.044	-3.853	11.179	1.00	30.33
ATOM	5456	0	LEU	696	48.006	-3.926	9.948		29.41
ATOM	5457	N	GLY	697	48.374	-2.738	11.831		30.92
ATOM	5459	CA	GLY	697	48.655	-1.503	11.113		30.35
	5460	C	GLY	697	47.420	-0.650	10.912		
ATOM	5461	0	GLY	697	47.359	0.178	10.000		30.65
ATOM	5462	N	GLY	698	46.428	-0.836	11.772		30.01
ATOM	5464	CA	GLY	698	45.209	-0.063			30.50
ATOM	5465		GLY	698	45.416	1.415			30.36
ATOM	5466	Ο.	GLY	698	46.320	1.809			30.07
ATOM	5467	N	SER	699	44.554	2.228			30.56
ATOM	5469	CA	SER	699	44.597	3.674			29.65
ATOM	5470	CB		699	44.263				28.42
ATOM	5471			699	43.960				24.61
ATOM	5473			699	43.621				31.25
ATOM	5474			699	42.406				8.27
					-2.200	3.930	12.474	1.00 2	7.14
CCCD/cc									

ATOM	5475	N	PRO	700	44.160	4.682	13.675	1.00	29.29
ATOM	5476	CD	PRO	700	45.587	4.867	13.999	1.00	26.09
MOTA	5477	CA	PRO	700	43.303	5.155	14.764	1.00	29.30
MOTA	5478	CB	PRO	700	44.319	5.624	15.812	1.00	27.68
MOTA	5479	CG	PRO	700	45.531	5.982	14.985	1.00	27.85
ATOM	5480	С	PRO	700	42.413	6.305	14.306	1.00	29.71
MOTA	5481	0	PRO	700	42.800	7.096	13.446	1.00	31.38
MOTA	5482	N	TYR	701	41.204	6.357	14.854	1.00	29.51
ATOM	5484	CA	TYR	701	40.246	7.419	14.548	1.00	30.25
MOTA	5485	CB	TYR	701	40.559	8.647	15.405	1.00	33.50
MOTA	5486	CG	TYR	701	40.321	8.413	16.866	1.00	37.84
ATOM	5487	CD1	TYR	701	41.323	8.638	17.803	1.00	40.05
ATOM	5488	CE1	TYR	701	41.092	8.412	19.158	1.00	42.28
MOTA	5489	CD2	TYR	701	39.084	7.965	17.310	1.00	41.54
MOTA	5490	CE2	TYR	701	38.845	7.738	18.653	1.00	43.70
ATOM	5491	CZ	TYR	701	39.845	7.963	19.574	1.00	42.63
ATOM	5492	ОН	TYR	701	39.584	7.716	20.907	1.00	45.31
MOTA	5494	C	TYR	701	40.173	7.829	13.088	1.00	28.45
ATOM	5495	0	TYR	701	40.356.	9.001	12.760	1.00	29.03
ATOM	5496	Ñ	PRO	702	39.901	6.867	12.191	1.00	28.05
ATOM	5497	CD	PRO	702	39.671	5.430	12.417	1.00	2690
ATOM ATOM	5498	CA	PRO	702	39.815	7.181	10.764	1.00	27.48
	5499	CB	PRO	702	39.610	5.807	10.119	1.00	27.06
ATOM ATOM	5500	CG	PRO	702	38.923	5.036	11.169	1.00	28.28
ATOM	5501 5502	C O	PRO	702	38.689	8.145	10.440	1.00	26.81
ATOM	5503	N	PRO GLY	702 703	37.554	7.953	10.865	1.00	26.26
ATOM	5505	CA	GLY	703	39.035 38.085	9.192 10.217	9.693	1.00	28.48
ATOM	5506	C	GLY	703	37.862	11.285	9.295 10.351	1.00	26.54
ATOM	5507	0	GLY	703	37.110	12.231	10.331	1.00	28.03 28.93
ATOM	5508	N	VAL	704	38.518	11.149	11.505	1.00	28.16
ATOM	5510	CA	VAL	704	38.369	12.081	12.619	1.00	29.55
ATOM	5511	СВ	VAL	704	38.473	11.360	13.984	1.00	28.50
ATOM	5512	CG1	VAL	704	38.330	12.350	15.135	1.00	28.07
ATOM	5513	CG2	VAL	704	37.403	10.295	14.091	1.00	29.78
ATOM	5514	C	VAL	704	39.375	13.227	12.588	1.00	32.00
ATOM	5515	0	VAL	704	40.578	13.028	12.758	1.00	33.85
ATOM	5516	N	PRO	705	38.888	14.446	12.336	1.00	33.56
MOTA	5517	CD	PRO	705	37.512	14.763	11.906	1.00	33.69
MOTA	5518	CA	PRO	705	39.745	15.628	12.280	1.00	32.65
MOTA	5519	CB	PRO	705	38.863	16.647	11.569	1.00	34.10
MOTA	5520	CG	PRO	705	37.478	16.256	12.021	1.00	36.38
ATOM	5521	С	PRO	705	40.164	16.081	13.668	1.00	33.22
MOTA	5522	0	PRO	705	39.549	15.708	14.668	1.00	33.26
MOTA	5523	N	VAL	706	41.198	16.912	13.710	1.00	34.61
MOTA	5525	CA	VAL	706	41.764	17.417	14.954	1.00	37.72
ATOM	5526	CB	VAL	706	42.803	18.527	14.673	1.00	39.14
MOTA	5527	CG1	VAL	706	43.483	18.941	15.957	1.00	39.12
ATOM	5528	CG2	VAL	706	43.836	18.038	13.670	1.00	41.07
ATOM	5529	C	VAL	706	40.740	17.934	15.969	1.00	38.70
MOTA	5530	0	VAL	706	40.761	17.536	17.136	1.00	38.42
MOTA	5531	N	GLU	707	39.834	18.796	15.517	1.00	40.43
MOTA	5533	CA	GLU	707	38.823	19.375	16.395	1.00	40.66
MOTA	5534	CB	GLU	707	37.973	20.379	15.621	1.00	43.40

	ATOM	F F 2 =					_	. •			
		5535	С	GĻU	707	37	940				
	ATOM	5536	0	GLU	707	٠, ٠	940	18	3.316	17.028	1.00 41.03
	ATOM	5537	N	GLU	708	37.	642	18	.370	18.231	
	MOTA	5539	CA	GLU.	708	37.	560	17		16.224	1.00 41.52
	ATOM	5540	CB	GLU		36.	708			16.700	1.00 41.62
	ATOM	5541	CG	GLU	708	36.	179			15.700	1.00 41.06
	ATOM	5542	CD		708	35.	281			15.523	1.00 45.19
	ATOM	5543		GLU	708	34.(		16		14.571	1.00 48.74
	ATOM	5544	OE1	GLU	708	33.5	523	10		5.258	1.00 57.18
	3		OE2	GLU	708	33.6	46			6.207	1.00 54.30
		5545	С	GLU	708	37.4	43		934 1	4.837	1.00 61.76
		5546	0	GLU	708	37.4	43		363 <sub>l</sub>	7.694	
		5547	N		709	36.8	67	14.	927 1		
	MOTA	554.9	CA		709	38.7		15.			1.00 36.76
	TOM S	5550	CB			39.5		14.	_	_	1.00 37.78
	TOM 9	5551	~~		709	41.00	07	14.			1.00 38.13
A	ma				709	41.98	34	13.9		7.820	1.00 35.45
					09	41.82		12.0		786	1.00 35.57
				LEU 7	09	43.40				.729	1.00 32.33
				LEU 7	09	39.55		13.9		.484 1	00 31.98
		555 (	o j	LEU 7	09	39.36		14.9	46 19		
			1		10			14.2	50 20		
		558 (	CA I		10	39.77		16.2	54 19		
	'OM 5	559 C			LO	39.80	7 :	16.9			
		60 C		HE 71		39.99	7 ]	18.4	75 20	_	.00 43.61
AT						41.328	3 1	8.8			.00 48.22
AT						42.395	1	7.93			.00 51.77
ATO	OM 55			HE 71		41.513	2	0.07	-		00 52.94
ATO	OM 55	<b>.</b> .		HE 71	0	43.632		8.27			00 53.99
ATO			_	IE 71	0	42.746					00 56.48
ATC		<b>-</b> -	Z PI	IE 71	0	43.807		0.42	-	021 1.	00 55.72
ATO		-	PI	E 71	0	38.519		9.51		069 1.	
ATO		•	PH			38.539	16	5.72	5 21.	796 1.	
	• •		LY				16	5.424	22.5		
ATO			LY			37.399	16	.804	21.0		
ATO		1 CB				36.095	.16	. 587	21.6		
ATO		2 CG	LY			34.977	16	.878	20.6		- • • •
ATOM		3 CD	LYS	_		33.601	16	. 765	21.2	_	
ATON	1 557					32.510	17	.206			. • •
ATOM	1 557		LYS			31.158	16	873		62 1.0	0 49.97
ATOM		<b>-</b>	LYS			30.038		412			0 51.70
ATOM	5580		LYS		3	35.986	16	. 412	20.19	50 1.0	0 57.55
ATOM		•	LYS		3	35.589		173	22.26	1.0	0 42.72
ATOM			LEU	712		6.392	_	999	23.42	0 1.00	41.16
ATOM			LEU	712	3	6.361		176	21,47	1 1.00	
ATOM			LEU	712	2	6 000	12.	770	21.89	8 1.00	
		CG	LEU	712	3	6.922	11.	843	20.80	9 1.00	
ATOM	5586	CD1	LEU	712	3	6.090	11.	528	19.56		
ATOM	5587	CD2	LEU		3	6.902	10.	620	18.63		
ATOM	5588	C	LEU	712	3	4.760	10.	868	19.95		
ATOM	5589	o		712	3,	7.158	12.5		22 22		
ATOM	5590		LEU	712	36	5.697	11.8	206	23.180	_	42.34
ATOM	5592	И	LEU	713	3 8	3.366	72 7	77	24.107	- •	40.77
ATOM		CA	LEU	713		.240	13.1	.ZI	23.208	1.00	42.68
ATOM	5593	CB	LEU	713	40	.581	13.0	25	24.371	1.00	44.05
	5594	CG	LEU	713	 /\ 1	. 201	13.7	10	24.100		
MOTA	5595	CD1	LEU	713	4.7	.418	13.1	14	22.963	1.00	45.45
ATOM	5596	CD2	LEU		42	.676	13.9	45	22.750		44.78
ATOM	5597	C	LEU	713	41	.757	11.6		23.282	1.00	41.89
			∪تدب	713	38	. 571	13.65		25.591	1.00	43.21
SSSD/55	145. vn1							•	~2.57[	1.00	44.66

ATOM 5599 N LYS 714 34 ATOM 5601 CA LYS 714 34 ATOM 5602 CB LYS 714 34 ATOM 5602 CB LYS 714 34 ATOM 5603 CG LYS 714 34 ATOM 5604 CD LYS 714 34 ATOM 5605 CE LYS 714 34 ATOM 5606 NZ LYS 714 34 ATOM 5610 C LYS 714 34 ATOM 5611 O LYS 714 34 ATOM 5611 O LYS 714 34 ATOM 5612 N GLU 715 34 ATOM 5615 CB GLU 715 34 ATOM 5616 CG GLU 715 34 ATOM 5616 CG GLU 715 34 ATOM 5617 CD GLU 715 34 ATOM 5618 OE1 GLU 715 34 ATOM 5620 C GLU 715 34 ATOM 5620 C GLU 715 34 ATOM 5621 O GLU 715 34 ATOM 5620 C GLU 715 36 ATOM 5620 C GLU 715 36 ATOM 5621 O GLU 715 36 ATOM 5620 N GLY 716 36 ATOM 5620 N HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5634 NPL HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5640 N ARG 718 36 ATOM 5641 CA ARG 718 36 ATOM 5642 CA ARG 718 36 ATOM 5645 CD ARG 718 36 ATOM 5646 NE ARG 718 36 ATOM 5646 NE ARG 718 36 ATOM 5647 NHI ARG 718 36 ATOM 5648 CZ ARG 718 36 ATOM 5648 CZ ARG 718 36 ATOM 5650 CA MET 719 39 ATOM 5650 CA MET 719 39 ATOM 5651 CG MET 719 30 ATOM 5652 CD MET 719 37 ATOM 5653 CE MET 719 37 ATOM 5655 CA MET 719 37 ATOM 5656 CA MET 719 37 ATOM 5650 CB MET 719 37 ATOM 5660 CB MET 719 37					
ATOM 5601 CA LYS 714 ATOM 5602 CB LYS 714 ATOM 5603 CG LYS 714 ATOM 5603 CG LYS 714 ATOM 5604 CD LYS 714 ATOM 5605 CE LYS 714 ATOM 5606 NZ LYS 714 ATOM 5610 C LYS 714 ATOM 5611 O LYS 714 ATOM 5612 N GLU 715 ATOM 5612 N GLU 715 ATOM 5614 CA GLU 715 ATOM 5615 CB GLU 715 ATOM 5616 CG GLU 715 ATOM 5616 CG GLU 715 ATOM 5617 CD GLU 715 ATOM 5619 OE2 GLU 715 ATOM 5620 C GLU 715 ATOM 5620 C GLU 715 ATOM 5624 CA GLY 716 ATOM 5625 C GLY 716 ATOM 5625 C GLY 716 ATOM 5626 O GLY 716 ATOM 5630 CB HIS 717 ATOM 5630 CB HIS 717 ATOM 5631 CG HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5638 C HIS 717 ATOM 5638 C HIS 717 ATOM 5638 C HIS 717 ATOM 5630 CB ARG 718 ATOM 5644 CA ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 NHI ARG 718 ATOM 5648 CZ ARG 718 ATOM 5656 O ARG 718 ATOM 5657 N MET 719 ATOM 5659 CA MET 719 ATOM 5650 CB MET 719 ATOM 5651 CG MET 719 ATOM 5652 NH ARG 718 ATOM 5655 CD ARG 718 ATOM 5650 CB MET 719 ATOM 5651 CG MET 719 ATOM 5652 NH ARG 718 ATOM 5655 CD ARG 718 ATOM 5660 CB MET 719	8.562 1	3.051	26.662	1.00	45.70
ATOM 5602 CB LYS 714 32 ATOM 5603 CG LYS 714 33 ATOM 5604 CD LYS 714 33 ATOM 5605 CE LYS 714 33 ATOM 5606 NZ LYS 714 33 ATOM 5606 NZ LYS 714 33 ATOM 5610 C LYS 714 33 ATOM 5611 O LYS 714 33 ATOM 5612 N GLU 715 33 ATOM 5614 CA GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5617 CD GLU 715 33 ATOM 5619 OE2 GLU 715 33 ATOM 5620 C GLU 715 33 ATOM 5620 C GLU 715 33 ATOM 5621 O GLU 715 33 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 ATOM 5633 ND1 HIS 717 36 ATOM 5634 CB HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5637 CB HIS 717 36 ATOM 5638 C HIS 717 36 ATOM 5639 O HIS 717 ATOM 5630 CB ATS 717 ATOM 5630 CB ATS 717 ATOM 5631 CG ATS 717 ATOM 5632 CD2 HIS 717 ATOM 5634 CB ARG 718 38 ATOM 5635 CE1 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5637 CB ARG 718 38 ATOM 5640 N ARG 718 38 ATOM 5641 CB ARG 718 38 ATOM 5645 CD ARG 718 38 ATOM 5646 NE ARG 718 38 ATOM 5646 NE ARG 718 30 ATOM 5657 N MET 719 38 ATOM 5659 CA MET 719 38 ATOM 5650 CB MET 719 38 ATOM 5650 CB MET 719 38 ATOM 5661 CG MET 719 38 ATOM 5662 SD MET 719 43	7.980 1	4.839	25.418	1.00	43.05
ATOM 5603 CG LYS 714 ATOM 5604 CD LYS 714 ATOM 5605 CE LYS 714 ATOM 5605 CE LYS 714 ATOM 5606 NZ LYS 714 ATOM 5610 C LYS 714 ATOM 5611 O LYS 714 ATOM 5611 O LYS 714 ATOM 5612 N GLU 715 ATOM 5615 CB GLU 715 ATOM 5616 CG GLU 715 ATOM 5616 CG GLU 715 ATOM 5617 CD GLU 715 ATOM 5619 OE2 GLU 715 ATOM 5619 OE2 GLU 715 ATOM 5620 C GLU 715 ATOM 5621 O GLU 715 ATOM 5622 N GLY 716 ATOM 5624 CA GLY 716 ATOM 5625 C GLY 716 ATOM 5626 O GLY 716 ATOM 5626 O GLY 716 ATOM 5627 N HIS 717 ATOM 5630 CB HIS 717 ATOM 5630 CB HIS 717 ATOM 5631 CG HIS 717 ATOM 5631 CG HIS 717 ATOM 5632 CD2 HIS 717 ATOM 5634 NA FIN 717 ATOM 5636 NE2 HIS 717 ATOM 5638 C HIS 717 ATOM 5639 O HIS 717 ATOM 5630 CB ARG 718 ATOM 5644 CG ARG 718 ATOM 5644 CG ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 NHI ARG 718 ATOM 5648 CZ ARG 718 ATOM 5648 CZ ARG 718 ATOM 5649 NHI ARG 718 ATOM 5640 NA RG 718 ATOM 5641 CB ARG 718 ATOM 5642 CA ARG 718 ATOM 5643 CB ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 NHI ARG 718 ATOM 5648 CZ ARG 718 ATOM 5649 NHI ARG 718 ATOM 5640 NA RG 718 ATOM 5641 CB ARG 718 ATOM 5642 CA ARG 718 ATOM 5643 CB ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 NHI ARG 718 ATOM 5648 CZ ARG 718 ATOM 5659 CA MET 719 ATOM 5650 CB MET 719 ATOM 5650 CB MET 719 ATOM 5651 CG MET 719 ATOM 5660 CB MET 719 ATOM 5660 CB MET 719 ATOM 5661 CG MET 719 ATOM 5663 CE MET 719 ATOM 5663 CE MET 719 ATOM 5665 CD MET 719 ATOM 5660 CB MET 719	7.300 1	5.510	26.524	1.00	42.19
ATOM 5604 CD LYS 714 33 ATOM 5605 CE LYS 714 33 ATOM 5606 NZ LYS 714 33 ATOM 5610 C LYS 714 33 ATOM 5611 O LYS 714 33 ATOM 5611 O LYS 714 33 ATOM 5612 N GLU 715 33 ATOM 5614 CA GLU 715 33 ATOM 5615 CB GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5617 CD GLU 715 33 ATOM 5618 OE1 GLU 715 33 ATOM 5619 OE2 GLU 715 33 ATOM 5620 C GLU 715 33 ATOM 5621 O GLU 715 33 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5634 CB HIS 717 36 ATOM 5635 CEI HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5640 N ARG 718 38 ATOM 5640 N ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5655 C ARG 718 40 ATOM 5655 C ARG 718 40 ATOM 5656 O ARG 718 40 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5650 CB MET 719 38 ATOM 5661 CG MET 719 38 ATOM 5662 SD MET 719 38 ATOM 5662 SD MET 719 43	6.884 1	6.921	26.127	1.00	42.41
ATOM 5605 CE LYS 714 ATOM 5606 NZ LYS 714 ATOM 5610 C LYS 714 ATOM 5611 O LYS 714 ATOM 5611 O LYS 714 ATOM 5612 N GLU 715 ATOM 5614 CA GLU 715 ATOM 5615 CB GLU 715 ATOM 5616 CG GLU 715 ATOM 5617 CD GLU 715 ATOM 5618 OE1 GLU 715 ATOM 5619 OE2 GLU 715 ATOM 5620 C GLU 715 ATOM 5621 O GLU 715 ATOM 5622 N GLY 716 ATOM 5624 CA GLY 716 ATOM 5625 C GLY 716 ATOM 5625 C GLY 716 ATOM 5626 O GLY 716 ATOM 5627 N HIS 717 ATOM 5630 CB HIS 717 ATOM 5631 CG HIS 717 ATOM 5631 CG HIS 717 ATOM 5632 CD2 HIS 717 ATOM 5633 ND1 HIS 717 ATOM 5634 CB HIS 717 ATOM 5635 CE1 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5638 C HIS 717 ATOM 5639 O HIS 717 ATOM 5630 CB ARG 718 ATOM 5644 CG ARG 718 ATOM 5644 CG ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 NHI ARG 718 ATOM 5648 CZ ARG 718 ATOM 5648 CZ ARG 718 ATOM 5648 CZ ARG 718 ATOM 5657 NHI ARG 718 ATOM 5658 CD ARG 718 ATOM 5658 CD ARG 718 ATOM 5659 CA MET 719 ATOM 5650 CB MET 719 ATOM 5650 CB MET 719 ATOM 5661 CG MET 719 ATOM 5662 SD MET 719 ATOM 5662 SD MET 719 ATOM 5663 CE MET 719 ATOM 5662 SD MET 719 ATOM 5663 CE MET 719 ATOM 5660 CB MET 719 ATOM 5660 CB MET 719 ATOM 5661 CG MET 719 ATOM 5662 SD MET 719 ATOM 5663 CE MET 719 ATOM 5663 CE MET 719 ATOM 5660 CB MET 719	8.076 1	7.828	25.918	1.00	46.10
ATOM 5606 NZ LYS 714 33 ATOM 5610 C LYS 714 36 ATOM 5611 O LYS 714 33 ATOM 5612 N GLU 715 33 ATOM 5614 CA GLU 715 33 ATOM 5615 CB GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5617 CD GLU 715 33 ATOM 5618 OE1 GLU 715 33 ATOM 5619 OE2 GLU 715 33 ATOM 5620 C GLU 715 33 ATOM 5621 O GLU 715 33 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 ATOM 5629 CA HIS 717 ATOM 5630 CB HIS 717 ATOM 5631 CG HIS 717 ATOM 5631 CG HIS 717 ATOM 5632 CD2 HIS 717 ATOM 5634 CH HIS 717 ATOM 5635 CE1 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5638 C HIS 717 ATOM 5639 O HIS 717 ATOM 5639 CA HIS 717 ATOM 5630 CB ARG 718 ATOM 5644 CG ARG 718 ATOM 5640 N ARG 718 ATOM 5640 N ARG 718 ATOM 5644 CG ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 NHI ARG 718 ATOM 5648 CZ ARG 718 ATOM 5648 CZ ARG 718 ATOM 5659 CA MET 719 ATOM 5650 CB MET 719 ATOM 5650 CB MET 719 ATOM 5661 CG MET 719 ATOM 5662 SD MET 719 ATOM 5662 SD MET 719 ATOM 5663 CE MET 719 ATOM 5663 CE MET 719 ATOM 5660 CB MET 719	7.684 1	9.259	25.589	1.00	49.86
ATOM 5610 C LYS 714 39 ATOM 5611 O LYS 714 39 ATOM 5612 N GLU 715 39 ATOM 5614 CA GLU 715 32 ATOM 5615 CB GLU 715 32 ATOM 5616 CG GLU 715 32 ATOM 5617 CD GLU 715 32 ATOM 5618 OE1 GLU 715 32 ATOM 5619 OE2 GLU 715 32 ATOM 5620 C GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5630 CB ARG 718 38 ATOM 5640 N ARG 718 38 ATOM 5640 N ARG 718 38 ATOM 5640 N ARG 718 38 ATOM 5640 NARG 718 39 ATOM 5650 CA ARG 718 39 ATOM 5650 CB MET 719 39 ATOM 5650 CB MET 719 39 ATOM 5660 CB MET 719 30 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	8.939 2	0.097	25.292	1.00	52.55
ATOM 5611 O LYS 714 33 ATOM 5612 N GLU 715 33 ATOM 5614 CA GLU 715 34 ATOM 5615 CB GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5616 CG GLU 715 33 ATOM 5618 OE1 GLU 715 33 ATOM 5619 OE2 GLU 715 33 ATOM 5620 C GLU 715 33 ATOM 5621 O GLU 715 33 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5630 CB HIS 717 36 ATOM 5631 CG HIS 717 36 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5634 CB HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 38 ATOM 5646 NE ARG 718 38 ATOM 5646 NE ARG 718 38 ATOM 5647 NH1 ARG 718 38 ATOM 5648 CZ ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 39 ATOM 5650 CB MET 719 ATOM 5661 CG MET 719 ATOM 5662 SD MET 719 ATOM 5662 SD MET 719 ATOM 5663 CE MET 719 ATOM 5663 CE MET 719 ATOM 5663 CE MET 719	9.889 2	0.148	26.459	1.00	50.17
ATOM 5612 N GLU 715 3: ATOM 5614 CA GLU 715 3: ATOM 5615 CB GLU 715 3: ATOM 5616 CG GLU 715 3: ATOM 5617 CD GLU 715 3: ATOM 5618 OE1 GLU 715 3: ATOM 5619 OE2 GLU 715 3: ATOM 5620 C GLU 715 3: ATOM 5621 O GLU 715 3: ATOM 5622 N GLY 716 3: ATOM 5624 CA GLY 716 3: ATOM 5625 C GLY 716 3: ATOM 5625 C GLY 716 3: ATOM 5627 N HIS 717 3: ATOM 5629 CA HIS 717 3: ATOM 5630 CB HIS 717 3: ATOM 5631 CG HIS 717 3: ATOM 5631 CG HIS 717 3: ATOM 5632 CD2 HIS 717 3: ATOM 5633 ND1 HIS 717 3: ATOM 5636 NE2 HIS 717 3: ATOM 5636 NE2 HIS 717 3: ATOM 5638 C HIS 717 3: ATOM 5639 O HIS 717 3: ATOM 5630 CB ARG 718 3: ATOM 5640 N ARG 718 3: ATOM 5641 CG ARG 718 3: ATOM 5642 CA ARG 718 3: ATOM 5644 CG ARG 718 3: ATOM 5645 CD ARG 718 4: ATOM 5646 NE ARG 718 4: ATOM 5647 NH1 ARG 718 3: ATOM 5648 CZ ARG 718 4: ATOM 5649 NH1 ARG 718 3: ATOM 5650 CB ARG 718 3: ATOM 5651 CD ARG 718 3: ATOM 5652 NH2 ARG 718 3: ATOM 5654 CD ARG 718 3: ATOM 5655 C ARG 718 3: ATOM 5650 CB MET 719 3: ATOM 5661 CG MET 719 3: ATOM 5662 SD MET 719 4: ATOM 5662 SD MET 719 4: ATOM 5663 CE MET 719 4: ATOM 5663 CE MET 719 4:	6.104 1	4.728	27.054	1.00	42.39
ATOM 5614 CA GLU 715 ATOM 5615 CB GLU 715 ATOM 5616 CG GLU 715 ATOM 5616 CG GLU 715 ATOM 5617 CD GLU 715 ATOM 5618 OE1 GLU 715 ATOM 5619 OE2 GLU 715 ATOM 5620 C GLU 715 ATOM 5621 O GLU 715 ATOM 5622 N GLY 716 ATOM 5624 CA GLY 716 ATOM 5625 C GLY 716 ATOM 5626 O GLY 716 ATOM 5627 N HIS 717 ATOM 5627 N HIS 717 ATOM 5630 CB HIS 717 ATOM 5630 CB HIS 717 ATOM 5631 CG HIS 717 ATOM 5631 CG HIS 717 ATOM 5632 CD2 HIS 717 ATOM 5633 ND1 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5638 C HIS 717 ATOM 5639 O HIS 717 ATOM 5639 O HIS 717 ATOM 5640 N ARG 718 ATOM 5641 CB ARG 718 ATOM 5644 CG ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 NH1 ARG 718 ATOM 5648 CZ ARG 718 ATOM 5648 CZ ARG 718 ATOM 5655 C ARG 718 ATOM 5657 N MET 719 ATOM 5659 CA MET 719 ATOM 5659 CA MET 719 ATOM 5650 CB MET 719 ATOM 5651 CG MET 719 ATOM 5652 SD MET 719 ATOM 5653 CE MET 719 ATOM 5653 CE MET 719 ATOM 5654 CB MET 719 ATOM 5655 CB MET 719 ATOM 5656 CB MET 719 ATOM 5656 CB MET 719 ATOM 5650 CB MET 719 ATOM 5660 CB MET 719	5.767 1	4.824	28.237	1.00	43.44.
ATOM 5615 CB GLU 715 32 ATOM 5616 CG GLU 715 32 ATOM 5617 CD GLU 715 32 ATOM 5618 OE1 GLU 715 32 ATOM 5619 OE2 GLU 715 32 ATOM 5620 C GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 ATOM 5622 N GLY 716 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 ATOM 5629 CA HIS 717 ATOM 5630 CB HIS 717 ATOM 5631 CG HIS 717 ATOM 5632 CD2 HIS 717 ATOM 5633 ND1 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5636 NE2 HIS 717 ATOM 5638 C HIS 717 ATOM 5639 O HIS 717 ATOM 5640 N ARG 718 ATOM 5641 CB ARG 718 ATOM 5642 CA ARG 718 ATOM 5642 CA ARG 718 ATOM 5643 CB ARG 718 ATOM 5644 CG ARG 718 ATOM 5645 CD ARG 718 ATOM 5646 NE ARG 718 ATOM 5646 NE ARG 718 ATOM 5647 CD ARG 718 ATOM 5648 CZ ARG 718 ATOM 5648 CZ ARG 718 ATOM 5649 NH1 ARG 718 ATOM 5649 NH1 ARG 718 ATOM 5655 C ARG 718 ATOM 5650 CB MET 719 ATOM 5661 CG MET 719 ATOM 5662 SD MET 719 ATOM 5663 CE MET 719	5.480 1	3.934	26.192	1.00	40.44
ATOM 5616 CG GLU 715 32 ATOM 5617 CD GLU 715 32 ATOM 5618 OE1 GLU 715 32 ATOM 5619 OE2 GLU 715 32 ATOM 5620 C GLU 715 32 ATOM 5620 C GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 32 ATOM 5631 CG HIS 717 32 ATOM 5632 CD2 HIS 717 32 ATOM 5633 ND1 HIS 717 32 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5638 C HIS 717 36 ATOM 5638 C HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5640 N ARG 718 38 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5655 C ARG 718 38 ATOM 5650 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 40 ATOM 5663 CE MET 719 40	4.342 1	3.118	26.593	1.00	37.90
ATOM 5617 CD GLU 715 32 ATOM 5618 OE1 GLU 715 32 ATOM 5619 OE2 GLU 715 32 ATOM 5620 C GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 32 ATOM 5630 CB HIS 717 32 ATOM 5631 CG HIS 717 32 ATOM 5632 CD2 HIS 717 32 ATOM 5633 ND1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 38 ATOM 5638 C HIS 717 38 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5640 N ARG 718 38 ATOM 5641 CB ARG 718 38 ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5647 CD ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5650 CA ARG 718 39 ATOM 5651 CD ARG 718 30 ATOM 5652 NH2 ARG 718 30 ATOM 5655 C ARG 718 30 ATOM 5656 CB MET 719 40 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	3.408 1	2.893	25.411	1.00	39.54
ATOM 5618 OE1 GLU 715 32 ATOM 5619 OE2 GLU 715 32 ATOM 5620 C GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5630 CB HIS 717 32 ATOM 5631 CG HIS 717 32 ATOM 5632 CD2 HIS 717 32 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5638 C HIS 717 32 ATOM 5638 C HIS 717 38 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 38 ATOM 5641 CG ARG 718 38 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5647 NH1 ARG 718 39 ATOM 5648 CZ ARG 718 40 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 42	2.800 1	4.174	24.846	1.00	45.20
ATOM 5619 OE2 GLU 715 32 ATOM 5620 C GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 36 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 32 ATOM 5631 CG HIS 717 32 ATOM 5632 CD2 HIS 717 32 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5638 C HIS 717 36 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 38 ATOM 5641 CB ARG 718 38 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5647 NH1 ARG 718 39 ATOM 5648 CZ ARG 718 40 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 42	2.032 1	3.936	23.563	1.00	47.85
ATOM 5620 C GLU 715 32 ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5638 C HIS 717 36 ATOM 5638 C HIS 717 37 ATOM 5638 C HIS 717 38 ATOM 5640 N ARG 718 38 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5647 NH1 ARG 718 39 ATOM 5648 CZ ARG 718 40 ATOM 5650 NH1 ARG 718 39 ATOM 5651 CD ARG 718 39 ATOM 5652 NH2 ARG 718 39 ATOM 5655 C ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5655 C ARG 718 39 ATOM 5655 C ARG 718 36 ATOM 5656 O ARG 718 36 ATOM 5655 C ARG 718 36 ATOM 5655 C ARG 718 36 ATOM 5656 CB MET 719 39 ATOM 5650 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	2.409 1	3.008	22.810	1.00	50.00
ATOM 5621 O GLU 715 32 ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5636 NE2 HIS 717 38 ATOM 5638 C HIS 717 38 ATOM 5638 C HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5640 N ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 38 ATOM 5646 NE ARG 718 38 ATOM 5646 NE ARG 718 40 ATOM 5647 NH1 ARG 718 39 ATOM 5648 CZ ARG 718 40 ATOM 5650 NH1 ARG 718 39 ATOM 5651 CD ARG 718 39 ATOM 5652 NH2 ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	1.061 14	4.677	23.304	1.00	50.41
ATOM 5622 N GLY 716 36 ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 38 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5640 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 38 ATOM 5646 NE ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5647 CD ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5650 CB ARG 718 39 ATOM 5651 CB ARG 718 39 ATOM 5652 NH2 ARG 718 38 ATOM 5655 C ARG 718 36 ATOM 5655 C ARG 718 36 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	4.793 13	1.773	27.157	1.00	37.31
ATOM 5624 CA GLY 716 36 ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5647 NH1 ARG 718 39 ATOM 5648 CZ ARG 718 40 ATOM 5650 NH2 ARG 718 39 ATOM 5651 C ARG 718 36 ATOM 5652 NH2 ARG 718 39 ATOM 5655 C ARG 718 36 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	3.970 10	0.907	27.450	1.60	36.79
ATOM 5625 C GLY 716 36 ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 35 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 36 ATOM 5638 C HIS 717 37 ATOM 5638 C HIS 717 38 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5640 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 40 ATOM 5650 NH2 ARG 718 39 ATOM 5651 C ARG 718 39 ATOM 5652 NH2 ARG 718 31 ATOM 5655 C ARG 718 31 ATOM 5655 C ARG 718 36 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	6.102 13	1.585	27.286	1.00	36.60
ATOM 5626 O GLY 716 36 ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 35 ATOM 5631 CG HIS 717 36 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5640 RARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 40 ATOM 5650 NH2 ARG 718 39 ATOM 5651 C ARG 718 31 ATOM 5652 NH2 ARG 718 31 ATOM 5655 C ARG 718 31 ATOM 5655 C ARG 718 31 ATOM 5656 O ARG 718 31 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	6.623 10	0.336	27.819	1.00	37.11
ATOM 5627 N HIS 717 36 ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 35 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5650 NH1 ARG 718 39 ATOM 5651 CA ARG 718 38 ATOM 5652 NH2 ARG 718 39 ATOM 5655 C ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	6.503	9.140	26.887	1.00	38.30
ATOM 5629 CA HIS 717 36 ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 35 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5650 NH1 ARG 718 39 ATOM 5651 C ARG 718 31 ATOM 5652 NH2 ARG 718 31 ATOM 5655 C ARG 718 31 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 43	6.603	7.994	27.34C	1.00	36.84
ATOM 5630 CB HIS 717 35 ATOM 5631 CG HIS 717 35 ATOM 5632 CD2 HIS 717 36 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5650 NH1 ARG 718 39 ATOM 5650 C ARG 718 38 ATOM 5651 C ARG 718 38 ATOM 5652 NH2 ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	6.307	9.404	25.592	1.00	40.24
ATOM 5631 CG HIS 717 34 ATOM 5632 CD2 HIS 717 34 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5646 NE ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5649 NH1 ARG 718 39 ATOM 5650 C ARG 718 38 ATOM 5651 C ARG 718 38 ATOM 5652 NH2 ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	5.167 8	8.353	24.579	1.00	42.63
ATOM 5632 CD2 HIS 717 34 ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5649 NH1 ARG 718 39 ATOM 5652 NH2 ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 43	5.800 8	8.951	23.217	1.00	43.13.
ATOM 5633 ND1 HIS 717 36 ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 37 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 40 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 39 ATOM 5650 NH1 ARG 718 39 ATOM 5651 C ARG 718 38 ATOM 5650 C ARG 718 38 ATOM 5650 C ARG 718 38 ATOM 5650 C ARG 718 38 ATOM 5651 C ARG 718 36 ATOM 5652 NH2 ARG 718 36 ATOM 5653 CARG 718 36 ATOM 5655 C ARG 718 36 ATOM 5656 CARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43	5.745	7.941	22.112	1.00	44.69
ATOM 5635 CE1 HIS 717 36 ATOM 5636 NE2 HIS 717 35 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5642 CA ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 40 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 39 ATOM 5652 NH1 ARG 718 39 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5663 CE MET 719 43	4.756	7.101	21.717	1.00	45.13
ATOM 5636 NE2 HIS 717 35 ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 40 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5650 NH1 ARG 718 39 ATOM 5651 C ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5663 CE MET 719 43	6.818	7.683	21.283	1.00	47.31
ATOM 5638 C HIS 717 37 ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 40 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5652 NH1 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 43	6.494 6	5.728	20.425	1.00	47.61
ATOM 5639 O HIS 717 38 ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 40 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 39 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5663 CE MET 719 43		5.35?	20.670	1.00	44.95
ATOM 5640 N ARG 718 37 ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5644 CG ARG 718 40 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 39 ATOM 5652 NH1 ARG 718 41 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 38 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5663 CE MET 719 43				1.00	44.84
ATOM 5642 CA ARG 718 38 ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 41 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 43				1.00	46.79
ATOM 5643 CB ARG 718 38 ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 41 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					45.44
ATOM 5644 CG ARG 718 38 ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 41 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					45.36
ATOM 5645 CD ARG 718 40 ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 39 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					43.82
ATOM 5646 NE ARG 718 40 ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 39 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 43					44.52
ATOM 5648 CZ ARG 718 40 ATOM 5649 NH1 ARG 718 39 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 40 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 42 ATOM 5662 SD MET 719 43					45.02
ATOM 5649 NH1 ARG 718 39 ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					43.12
ATOM 5652 NH2 ARG 718 41 ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					44.77
ATOM 5655 C ARG 718 38 ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					44.67
ATOM 5656 O ARG 718 36 ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					46.39
ATOM 5657 N MET 719 39 ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					45.94
ATOM 5659 CA MET 719 38 ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					47.59
ATOM 5660 CB MET 719 40 ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					45.34
ATOM 5661 CG MET 719 40 ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					44.28
ATOM 5662 SD MET 719 42 ATOM 5663 CE MET 719 43					42.30
ATOM 5663 CE MET 719 43					38.44
					36.97
ATOM 2004 C MET 719 38					36.09
ATOM ECCE O MEM BIG					46.21
					43.29
					48.79
ATOM 5668 CA ASP 720 37	.069 -0	0.063 2	0.666	1.00	48.87

							2	78						
	ATOM	5669	CB	ASP	720	3.6								
	ATOM	5670	CG	ASP	720	36	.099		.369	19.	513	1.00		•
	ATOM	5671	OD1	ASP	720		. 766		. 374		632	1.00	~	
	ATOM	5672	OD2	ASP	720		.762		. 583		981	1.00		
	<b>&gt;</b> - · ·	5673	C	ASP	720	33,	. 716		. 259		354	1.00		
		5674	0	ASP	720	38.	126		154		688	1.00		
		5675	N	LYS	721	39.	213		992	20.		1.00	46.1	
		5677	CA	LYS	721	37.	788		272	21.	322	1.00	44.1	
		678	CB		721	30.	689		413	21.4	104	1.00	45.2	
		679	CG		721	38.	172	-4.		22.4		1.00	43.2	
		680	CD	•	721	39.	072	-5.		22.5		1.00	42.0	
			CE	T	721	38.6	502	-6.	576	23.6		1.00	46.5	
		682			721	38.3	300	-7.9		23.1		1.00	49.96	
			_	<b>-</b>	721	37.9	37	8.5		24.2	40	1.00	51.80	
	Mar		o 1		21	38.7	69	-4.0	55	20.0		1.00	56.08	3
				•	22	37.7	36	-4.3	13	19.3		1.00	43.67	
					22	39.9	_	-4.2	33	19.5		1.00	44.02	
					22	41.2	_	-3.7	11 ;	20.00		1.00	43.94	
		91 (			22	40.1	_	-4.8	53 1	18.19		1.00	45.90	
		92 C			22	41.66		-4.7	20 1	7.94			43.96	
AT					22	42.04	16 .	-3.50		8.71			43.11	
AT		94 O		RO 72		39.77		6.31	17 1	8.29			45.16	
ATO		95 N		ER 72		39.76		6.88	18	9.38		•	43.09	
ATO		97 C	_	ER 72		39.38		6.90	2 1	7.3.7			41.32	
ATC				_		39.04		9.31	6 1	7.14			45.79	
ATC	_			. –		38.30		8.66	4 1	5.35			16.67	
ATO		)1 C	SE			39.13		8.41	4 14	1.736			4.69	
ATO		_	SE			40.42		8 . 96	1 17	7.148			9.79	
ATO	0	3 N	AS			41.360		9.41	1 16	. 581			6.90	
ATO						40.540		0.131	l 17	.760			8.81	
ATO		-~				41.826		0.804	1.7	. 849		_	9.28	
ATOM						42.480		.947	. 16	.469		00 5	2.10	
ATON		:	l Asi			41.774		. 957	15	. 592	1.		5.86 3.72	
ATOM			2 Ash			41.686 41.258		.140	15	.941	1.0		2.28	
ATOM			ASN			42.665	_	.503		.449	1.0		3.56	
ATOM ATOM			ASN			43.621		. 931	18.	770	1.0		97	
ATOM			CYS			42.202	- 9	. 274	18.	369	1.0		. 85	
ATOM			CYS			42.853		.859	20.	004	1.0		. 02	
ATOM		CB	CYS		4	12.708	- 9	094	21.	049	1.0		.18	
	5718	SG	CYS	725		13.424	-7.	583	20.	811	1.0		. 75	
ATOM ATOM	5719	C	CYS	725	4	2.131	-6.	577	22.	130	1.0		. 75 . 37	
ATOM		0	CYS	725	4	0.916	-9.	507	22.	315	1.0			
ATOM	5721	N	THR	726	4	2.866	-9.	371	22.4	417	1.0			
	5723	CA	THR	726	4	2.262	-10.	880	23.2	249	1.00			
ATOM	5724	CB	THR	726	4	3.251	-10.	541	24.4	190	1.00			
ATOM	5725	OG1	THR	726	4	4 226	-11.	444	25.2		1.00			
ATOM	5727	CG2	THR	726	4.	4.236	-10.6	548	25.9	76	1.00			
ATOM	5728	С	THR	726	4.	3.982	-12.3	363	24.3	52	1.00			
ATOM	5729	0	THR	726	4.	L.788	-9.3	869	25.3		1.00			
ATOM	5730	N	ASN	727	42	3.305	-8.2	56	25.2		1.00		93 	
ATOM	5732	CA	ASN	727	40	.829	-9.6	22	26.2		1.00		5	
ATOM	5733	CB	ASN	727	40	.335	-8.5	77	27.1	_	1.00	50.4		
ATOM	5734	CG	ASN	727	39	.190	-9.0	99	28.0		1.00	52.1	17	
ATOM	5735	OD1	ASN	727	39	.533	-10.4	09	28.71		1.00	57.5	7	
				121	40	.709	-10.7		28.83		1.00	66.4		
SSSD/551	145. v01											70.4	3	

ATOM	5736	ND2	ASN	727	38.500	-11.122	29.175	1.00	68.43
MOTA	5739	С	ASN	727	41.491	-8.091	28.023	1.00	50.29
ATOM	5740	0	ASN	727	41.467	-6.976	28.540	1.00	49.88
ATOM	5741	N	GLU	728	42.518	-8.927	28.163	1.00	50.60
ATOM	5743	CA	GLU	728	43.700	-8.597	28.956	1.00	49.33
ATOM	5744	CB	GLU	728	44.529	-9.859	29.220	1.00	50.44
MOTA	5745	CG	GLU	728	45.802	-9.600	30.008	1.00	55.30
ATOM	5746	CD	GLU	728	46.577	-10.862	30.354	1.00	57.40
ATOM	5747	OE1	GLU	728	46.716	-11.754	29.489	1.00	<b>56.7</b> 5
ATOM	5748	OE2	GLU	728	47.062	-10.950	31.502	1.00	59.85
MOTA	5749	С	GLU	728	44.539	-7.552	28.212	1.00	47.08
ATOM	5 <b>7</b> 50	0	GLU	728	44.888	-6.512	28.776	1.00	48.02
MOTA	5751	N	LEU	729	44.846	-7.821	26.945	1.00	43.34
MOTA	5753	CA	LEU	729	45.630	-6.891	26.129	1.00	42.01
MOTA	5754	CB	LEU	729	45.899	-7.500	24.751	1.00	39.46
ATOM	5755	CG	LEU	729	46.911	-8.639	24.772	1.00	40.31
ATOM	5756	CD1	LEU	729	46.782	-9.482	23.531	1.00	42.21
ATOM	5757	CD2	LEU	729	48.314	-8.068	24.900	1.00	42.49
ATOM	5758	С	LEU	729	44.901	-5.557	25.980	1.00	40.61
ATOM	5759	0	LEU	729	45.510	-4.481	25.953	1.00	38.33
ATOM	5760	N	TYR	730	43.580	-5.637	25.909	1.00	39.07
ATOM	5762	CA	TYR	730	42.761	-4.455	25.773	1.00	38.61
ATOM	5763	CB	TYR	730	41.341	-4.837	25.369	1.00	36.79
ATOM	5764	CG	TYR	730	40.454	-3.646	25.125	1.00	37.08
ATOM	5765	CD1	TYR	730	40.760	-2.721	24.127	1.00	32.86
ATOM	5766	CE1	TYR	730	39.961	-1.616	23.912	1.00	29.79
MOTA	5767	CD2	TYR	730	39.328	-3.420	25.91€	1.00	36.99
ATOM	5768	CE2	TYR	730	38.522	-2.312	25.704	1.00	36.69
MOTA	5769	CZ	TYR	730	38.853	-1.412	24.706	1.00	32.69
MOTA	5770	ОН	TYR	730	38.044	-0.320	24.492	1.00	38.80
ATOM	5772	С	TYR	730	42.767	-3.662	27.080	1.00	39.75
MOTA	5773	0	TYR	730	42.781	-2.430	27.065	1.00	40.53
ATOM	5774	N	MET	731	42.738	-4.360	28.210	1.00	41.88
ATOM	5776	CA	MET	731	42.778	-3.684	29.509	1.00	45.34
ATOM	5777	CB	MET	731	42.658	-4.697	30.646	1.00	53.46
MOTA	5778	CG	MET	731	41.253	-5.248	30.836	1.00	64.30
ATOM	5779	SD	MET	731	40.134	-4.095	31.653	1.00	75.78
MOTA	5780	CE	MET	731	40.657	-4.338	33.370	1.00	69.70
ATOM	5781	С	MET	731	44.099	-2.927	29.614	1.00	41.53
ATOM	5782	0	MET	731	44.157	-1.814	30.138	1.00	37.91
ATOM	5783	N	MET	732	45.156	-3.545	29.098	1.00	40.48
ATOM	5785	CA	MET	732	46.478	-2.937	29.091	1.00	40.23
ATOM	5786	CB	MET	732	47.508	-3.872	28.436	1.00	40.29
MOTA	5787	CG	MET	732	48.929	-3.307	28.390	1.00	38.07
MOTA	5788	SD	MET	732	50.171	-4.522	27.908	1.00	37.65
MOTA	5789	CE	MET	732	50.407	-5.343	29.431	1.00	37.90
MOTA	5790	С	MET	732	46.378	-1.623	28.317	1.00	38.96
MOTA	5791	0	MET	732	46.843	-0.591	28.790	1.00	41.36
ATOM	5792	N	MET	733	45.744	-1.663	27.148	1.00	36.94
MOTA	5794	CA	MET	733	45.574	-0.463	26.340	1.00	35.19
MOTA	5795	СВ	MET	733	44.796	-0.769	25.070	1.00	36.07
ATOM	5796	CG	MET	733	45.549	-1.577	24.048	1.00	35.99
ATOM	5797	SD	MET	733	44.471	-1.851	22.641	1.00	40.05
MOTA	5798	CE	MET	733	45.244	-3.351	21.909	1.00	33.13
									JJ.1J

							28	30				
	ATOM	5799	C	MET	700							
	ATOM	5800	0		733		. 800	0	.560	27 343		
	ATOM	5801	N	MET	733	45.	207	1	.719	27.141	1.00	37.29
	MOTA	5803	CA	ARG	734	43.	690		.125	27.245	1.00	39.14
	ATOM	5804		ARG	734	42.	849			27.735	1.00	38.76
	ATOM	5805	CB	ARG	734		577		.014	28.532	1.00	39.49
	ATOM		CG	ARG	734	40.			. 297	28.993	1.00	40.33
	ATOM	5806	CD	ARG	734	40.			225	27.856	1.00	
	ATOM	5807	NE	ARG	734	30.	436	0.	877	26.909	_	38.02
	3.00	5809	CZ	ARG	734	39.4	443	1.		27.567	_	42.72
	7	5810	NH1	ARG	734	38.5	120	1.		27.700		48.85
		5813	NH2	ARG	734	37.4	135	0.		27.222		52.35
		5816	C	ARG		37.4				28.338		54.79
	ATOM .	5817	0	ARG	734	43.6				<b>`</b> -		54.69
	TOM !	5818	N		734	43.4	45	2.7		0000	1.00 . 3	88.70
A		5820	CA	ASP	735	44.5	30	0.7		0.068	1.00 4	0.92
А	An		~-	ASP	735	45.3	79	1.2		0.276		8.76
					735	46.32	25			1.399		8.60
			<b>~</b>		735	45.62		0.0		1.825		1.34
				ASP	735	46.04		-1.0		2.574 j		4.66
	Da			ASP ·	735	44.65		2.1	94 3:			
			C ;	ASP 7	735	46.00	_	0.7	13 3:	_		3.15
			) ;		735	46.21	_	2.38	35 30			1.46
		327 N	1 (		36	46.23	5	3.44				7.76
		329 C	:A (		36	46.89	0	2.18		_	_	.35
	OM 58	130 C			36	47.73		3.19				.39
AT		31 S				48.379	9 :	2.65				.77
AT	-	32 C			36	49.453	} :	1.26				.62
ATO			_		36	46.938	4	1.42			00 30	. 96
ATC	DM 58:		_		36	47.516		6.49	_		00 35	. 98
ATC	DM 58:				<b>3</b> 7 <sub>.</sub>	45.620		. 29			00 37.	38
ATC	M 583	37 CE		RP 73		44.772		.423	•		00 38.	50
ATO	M 583		<b></b>			43.791	_	.028		370 l.	00 40.	
ATO	M 583	_			7	44.453				271 1.	00 38.	41
ATO		_		. •	7	43.893		- 586	- •	011 1.	00 39.	33
ATO		_		P 73	7	44.852		.718		020 1.0		
ATO		_ `		P 73	7	42.672		.583	23.		00 39.	
ATON				P 73		45.695		040	24.5	900 1.0		
ATOM			1 TR			45.941		932	25.5	556 1.0		
ATOM			2 TRI	737	,	14 622		336	24.3			
	-010		TRE			44.627		795	22.8	59 1.0		1
ATOM	-01,		TRE	737	7	12.452		261	23.7	78 1.0		
ATOM		C	TRE		•	3.426	2.	145	22.7	72 1.0		
ATOM		0	TRP		-	4.028	6.6	029	29.5			
ATOM		N	HIS	,	-	2.979		558	29.3			0
ATOM		CA	HIS		4	4.575		373	30.76			
ATOM	5853	СВ			4	3.932	6.4		21 0			
ATOM	5854	CG	HIS	738	4	4.454	5.7		31.94	-	44.64	
ATOM	5855	CD2	HIS	738	4.	3.742	6.1		33.20		46.20	
ATOM	5856		HIS	738	4:	3.473	7.3	20	34.45		50.35	
ATOM	5858	ND1	HIS	738	43	3.220	7.3	19	34.96	3 1.00		
ATOM		CEI	$\mathtt{HIS}$	738	42	.659	5.2	44	35.35	5 1.00	49.94	
ATOM	5859	NE2	HIS	738	42	.798	5.8		36.35	7 1.00	52.92	
	5861	C	HIS	738	11	174	7.19		36.14	6 1.00		
ATOM	5862	0	HIS	738	44	.174	7.92	21	32.03	7 1.00	46.91	
ATOM	5863	N	ALA	739	45	.314	8.35		32.02		45.26	
ATOM	5865	CA	ALA		43	.099	8.68	6	32.224	-	45.31	
ATOM	5866	CB	ALA	739	43	.155	10.15		32.322		46.61	
				739	41	. 823	10.68		32.790		48.49	*
SSSD/55	145. v()1						_	•		1.00	49.69	
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ATOM	5867	C	ALA	739	44.272	10.682	33.224	1.00	50.77
ATOM	5868	0	ALA	739	45.004	11.601	32.846	1.00	51.77
ATOM	5869	N	VAL	740	44.336	10.138	34.439	1.00	51.47
ATOM	5871	CA	VAL	740	45.352	10.485	35.439	1.00	51.09
ATOM	5872	CB	VAL	740	44.897	10.075	36.850	1.00	52.40
MOTA	5873	CG1	VAL	740	45.847	10.624	37.878	1.00	53.38
MOTA	5874	CG2	VAL	740	43.485	10.544	37.105	1.00	55.18
ATOM	5875	C	VAL	740	46.649	9.727	35.130	1.00	48.99
ATOM	5876	0	VAL	740	46.773	8.534	35.440	1.00	47.72
ATOM	5877	N	PRO	741	47.646	10.421	34.565	1.00	48.31
ATOM	5878	CD	PRO	741	47.603	11.861	34.253	1.00	47.84
ATOM	5879	CA	PRO	741	48.949	9.852	34.197	1.00	48.51
MOTA	5880	CB	PRO	741	49.762	11.087	33.828	1.00	46.83
MOTA	5881	CG	PRO	741	48.714	1.2.000	33.255	1.00	46.21
ATOM	5882	C	PRO	741	49.641	9.016	35.275	1.00	49.12
MOTA	5883	O	PRO	741	50.449	8.139	34.955	1.00	46.57
ATOM	5884	N	SER	742	49.327	9.290	36.541	1.00	49.47
ATOM	5886	CA	SER	742	49.928	8.557	37.651	1.00	49.50
ATOM	5887	CB	SER	742	49.760	9.326	38.963	1.00	51.06
MOTA	5888	OG	SER	742	48.403	9.638	39.209	1.00	53.81
ATOM	5890	C	SER	742	49.339	7.159	37.787	1.00	48.81
ATOM	5891	0	SER	742	49.926	6.284	38.427	1.00	49.45
ATOM	5892	N	GLN	743	48.164	6.959	37.203	1.00	47.82
ATOM	5894	CA	GLN	743	47.529	5.658	37.273	1.00	46.34
ATOM	5895	CB	GLN	743	46.022	5.791	37.432	1.00	49.74
ATOM	5896	CG	GLN	743	45.519	5.305	38.784	1.00	55.41
MOTA	5897	C:D	GLN	743	46 178	5.030	39.947	1.00	59.15
MOTA	5898	OE1	GLN	743	46.905	5.425	40.748	1.00	59.02
MOTA	5899	NE2	GLN	743	45.922	7.338	40.052	1.00	60.03
ATOM	5902	С	GLN	743	47.874	4.768	36.095	1.00	44.34
ATOM	5903	0	GLN	743	47.548	3.578	36.114	1.00	44.64
MOTA	5904	N	ARG	744	48.497	5.339	35.059	1.00	42.83
ATOM	5906	CA	ARG	744	48.914	4.559	33.880	1.00	40.34
ATOM	5907	CB	ARG	744	49.349	5.469	32.724	1.00	35.84
MOTA	5908	CG	ARG	744	48.296	6.406	32.190	1.00	28.25
ATOM	5909	CD	ARG	744	48.906	7.383	31.216	1.00	22.56
ATOM	5910	NE	ARG	744	47.948	8.437	30.922	1.00	28.09
ATOM	5912	CZ	ARG	744	48.258	9.658	30.493	1.00	32.83
MOTA	5913	NH1	ARG	744	49.524	10.001	30.278	1.00	34.44
ATOM	5916	NH2	ARG	744	47.307	10.569	30.360	1.00	32.00
ATOM	5919	С	ARG	744	50.110	3.712	34.295	1.00	41.58
MOTA	5920	0	ARG	744	50.906	4.124	35.145	1.00	45.48
ATOM	5921	N	PRO	745	50.223	2.489	33.754	1.00	40.97
ATOM	5922	CD	PRO	745	49.345	1.749	32.831	1.00	39.90
ATOM	5923	CA	PRO	745	51.381	1.685	34.157	1.00	39.77
ATOM	5924	CB	PRO	745	51.063	0.311	33.558	1.00	39.31
MOTA	5925	CG	PRO	745	50.255	0.642	32.344	1.00	40.98
MOTA	5926	C	PRO	745	52.664	2.269	33.573	1.00	38.44
ATOM	5927	0	PRO	745	52.631	3.009	32.595	1.00	39.64
MOTA	5928	N	THR	746	53.783	2.001	34.224	1.00	37.50
ATOM	5930	CA	THR	746	55.066	2.462	33.728	1.00	37.56
ATOM	5931	CB	THR	746	56.108	2.571	34.869	1.00	38.58
MOTA	5932	OG1	THR	746	56.286	1.285	35.487	1.00	43.28
MOTA	5934	CG2	THR	746	55.666	3.567	35.899	1.00	34.64

ATOM				202			
ATOM 593		THR 746	5 55 5	1.0			
ATOM 593	6 0	THR 746	00.5		393 32	. 739	1.00 36.49
ATOM 593	7 N	PHE 747			234 32		
ATOM 593			20.4	53 1.			
ATOM 594	_		30.5	950.		_	
ATOM 594	. ~~		58.02				1.00 33.48
ATOM 594		PHE 747	57.41	_			1.00 34.35
ATOM 594		PHE 747	56.71		•	920	1.00 32.49
ATOM 5944		PHE 747	57.51	•	-	856 ]	1.00 30.69
		HE 747	56.12	_		018 1	1.00 32.81
	F	HE 747	56.92				00 29.41
2	CZ p	HE 747	56.22				.00 32.93
ATOM 5947	C P	HE 747	50.22				
ATOM 5948	O <b>p</b>	HE 747	57.62		63 31.6		
ATOM 5949			57.616	-1.4	74 31.0		
ATOM 5951	CA L		58.142	-0.1	28 32.8		
ATOM 5952			58.748	-1.20	05 33.5		.00 37.75
ATOM 5953			59.382	-0.66	_		.00 39.67
ATOM 5954			59.958	-1.75			.00 43.06
ATOM 5955	CD LY		60.750	-1.20			00 48.96
30000	CE LY		61.183			66 1.	00 52.20
	NZ LY	S 748	62.057	-2.34			00 53.62
3 mass	C LY	S 748	57.680	-1.89		31 1.	00 54.82
	O LY		57.902	-2.26		32 1.	
ATOM 5962	N GLI		57.902	-3.45		2 1.	
ATOM 5964	CA GL		56.503	-1.818	34.33	1 1.0	
ATOM 5965	CB GLM		55.402	-2.742	34.62		
ATOM 5966	CG GLN		54.177	-1.991	35.14		
ATOM 5967	CD GLN		54.395	-1.149	36.37	_	
ATOM 5968	OE1 GLN	3	53.175	-0.304			
ATOM 5969	NE2 GLN		53.272	0.914			
ATOM 5972			52.012	-0.940			
ATOM 5973			55.009	-3.455		0	
ATOM CO-		749	54.903	-4.679		_	
ATOM FORE	N LEU	750	54.802	.2.666			0 40.26
ATOM DOD	CA LEU	750	54.400		32.278		0 39.18
ATOM	CB LEU	750	54.369	-3.171	30.964	1.00	36.65
30000	G LEU	750	53.355	-2.039	29.927	1.00	34.58
ATOM	D1 LEU	750	53.644	-0.910	30.116	1.00	32.52
	D2 LEU	750	51.947	0.210	29.125	1.00	31.67
ATOM 5981	LEU	750	55.347	-1.435	29.935	1.00	
ATOM 5982 C	LEU		55.321	-4.255	30.477	1.00	
ATOM 5983 N			54.856	~5.267	29.963	1.00	
ATOM 5985 C	_		56.626	-4.035	30.620	1.00	35.81
ATOM 5986 C			57.607	-5.029	30.193	1.00	37.38
ATOM 5987 C	31 VAL	751	59.077	-4.545	30.411		38.66
ATOM		751	60.075	-5.646	30.041	1.00	35.42
ATOM 5989 C	- <del></del>	751	59.342	-3.324	29.559	1.00	29.83
ATOM FOR	VAL	751	57.337	-6.314		1.00	29.95
ATOM	VAL	751		-7.401	30.974	1.00	41.63
ATOM 5000	GLU			-6 174	30.396	1.00	42.43
ATOM TO			· <b>-</b>	-6.174	32.267	1.00	43.35
ATOM					33.111	1.00	47.39
ATOM 5995 CG	_		-	-6.914	34.587	1.00	50.66
ATOM 5996 CD			7.950	-6.243	35.101	1.00	
ATOM 5997 OE			8.006 .	-6.101	36.612	1.00	54.77
ATOM 5998 OF		_	8.246 .		37.102		55.14
ATOM 5999 C		752 5·	7.844 _		37.308	1.00	54.14
	310	752 5	5.496 _		32.655	1.00	57.73
SSSD/55145, v01						1.00	46.00



ATOM	6000	0	GLU	752	55.548	-9.261	32.328	1.00	46.25
MOTA	6001	N	ASP	753	54.380	-7.346	32.601	1.00	44.35
MOTA	6003	CA	ASP	753	53.099	-7.912	32.180	1.00	44.19
ATOM	6004	CB	ASP	753	52.059	-6.814	31.985	1.00	46.22
ATOM	6005	CG	ASP	753	51.512	-6.279	33.278	1.00	50.48
ATOM	6006	OD1	ASP	753	51.396	-7.062	34.248	1.00	52.15
MOTA	6007	OD2	ASP	<b>75</b> 3	51.170	-5.069	33.306	1.00	52.20
ATOM	6008	С	ASP	753	53.244	-8.608	30.849	1.00	44.54
ATOM	6009	0	ASP	753	52.770	-9.724	30.674	1.00	46.03
MOTA	6010	N	LEU	754	53.880	-7.918	29.906	1.00	44.43
ATOM	6012	CA	LEU	754	54.079	-8.438	28.563	1.00	43.70
ATOM	6013	CB	LEU	754	54.570	-7.339	27.618	1.00	43.48
ATOM	6014	CG	LEU	754	53.481	-6.350	27.201	1.00	44.67
ATOM	6015	CD1	LEU	754	54.095	-5.218	26.399	1.00	44.51
ATOM	601.6	CD2	LEU	754	52.384	-7.069	26.408	1.00	42.07
ATOM	6017	С	LEU	754	54.993	-9.642	28.512	1.00	43.14
MOTA	6018	0	LEU	754	54.795	-10.536	27.697	1.00	41.32
ATOM	6019	N	ASP	755	55.990	-9.671	29.383	1.00	44.74
MOTA	6021	CA	ASP	755	56.897	-10.800	29.426	1.00	47.24
ATOM	6022	CB	ASP	755	57.942	-10.575	30.517	1.00	51.26
ATOM	6023	CG	ASP	755	59.121	-11.518	30.407	1.00	55.39
ATOM	6024	OD1	ASP	755	59.739	-11.793	31.455	1.00	60.61
ATOM	6025	OD2	ASP	755	59.443	-11.970	29.283	1.00	57.16
ATOM	6026	C.	ASP	755	56.023	-12.005	29.771	1.00	47.67
ATOM	6027	0	ASP	755	56.041	-13.032	29.081	1.00	45.99
MOTA	6028	N	ARG	756	55.186	-11.816	30.789	1.00	46.72
MOTA	6030	CA	ARG	756	54.272	-12.851	31.256	1.00	46.25
ATOM	6031	CB	ARG	756	53.519	-12.368	32.499	1.00	46.31
MOTA	6032	CG	ARG	756	52.391	-13.287	32.953	1.00	46.99
ATOM	6033	CD	ARG	756	51.733	-12.776	34.227	1.00	48.10
MOTA	6034	NE	ARG	756	51.320	-11.379	34.118	1.00	53.67
ATOM	6036	CZ	ARG	756	50.294	-10.951	33.385	1.00	55.35
ATOM	6037	NHl	ARG	756	49.562	-11.812	32.684	1.00	54.10
ATOM	6040	NH2	ARG	756	50.008	-9.654	33.344	1.00	56.02
ATOM	6043	С	ARG	756	53.282	-13.261	30.175	1.00	45.05
MOTA	6044	0	ARG	756	53.213	-14.429	29.806	1.00	47.19
ATOM	6045	N	ILE	757	52.550	-12.289	29.647	1.00	43.47
ATOM	6047	CA	ILE	757	51.552	-12.553	28.617	1.00	43.80
MOTA	6048	CB	ILE	757	50.842	-11.241	28.161	1.00	42.02
ATOM	6049	CG2	ILE	757	49.811	-11.536	27.086	1.00	39.63
ATOM	6050	CG1	ILE	757	50.154	-10.578	29.361	1.00	40.00
MOTA	6051	CD1	ILE	757	49.600	-9.212	29.086	1.00	42.68
ATOM	6052	C	ILE	757	52.148	-13.296	27.428	1.00	46.03
MOTA	6053	0	ILE	757	51.549	-14.250	26.947	1.00	47.78
MOTA	6054	N	VAL	758	53.359	-12.925	27.015	1.00	49.03
ATOM	6056	CA	VAL	758	54.015	-13.584	25.884	1.00	51.51
MOTA	6057	CB	VAL	758	55.412	-12.971	25.556	1.00	50.75
ATOM	6058	CG1	VAL	758	56.105	-13.780	24.470	1.00	50.31
MOTA	6059	CG2	VAL	758	55.269	-11.541	25.081	1.00	52.52
ATOM	6060	С	VAL	758	54.209	-15.050	26.212	1.00	54.30
MOTA	6061	0	VAL	758	53.991	-15.915	25.369	1.00	54.80
ATOM	6062	N	ALA	759	54.617	-15.311	27.450	1.00	57.65
MOTA	6064	CA	ALA	759	54.858	-16.667	27.919	1.00	60.62
ATOM	6065	СВ	ALA	759	55.423	-16.637	29.327	1.00	60.32

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ATOM 6066 C ALA 759 53.50	
ATOM 6067 O 33 53.571 -17 470	
ATOM 6060 - ALA 759 53 568 - 776 27.889 1.00 63 36	
ATOM 6070 TEU 760 52 475 10.638 27.478 1.00 65 01	
760 54 10.856 28.305 1 05	
MON CB LEU 760 50 -17.533 28.333 1 00	
750 LEU 760 51.912 29.407 1	
CD1 LEU 760 "16.962 30 820	
49.988 -16.246 31 800 65.62	
31.109 -18 410 31.00 64.75	
ATOM 6076 O 150 50.483 -17.535 31.22/ 1.00 66.65	
ATOM 6077 N 700 49.390 18.080 26.984 1.00 64.89	
ATOM 5079 00 110 761 51 103 16 20.860 1.00 55 27	
ATOM 6080 CD THR 761 50.516 15.933 25.973 1.00 55.34	
THR 751 16.882 24.634 1 3.24	
Arrow OG1 THR 761 15.539 23.925 1 04.44	
ATTOM CG2 THR 761 -14.463 24.669	
50.249 -15 526 00 1.00 62.70	
51.003 -18.044 33 -1.00 60.59	
ATOM 6086 SG CVS 152.202 -18.201 23.769 1.00 64.71	
ATOM 5087 00 18 536 0 23.333 1.00 64 70	
ATOM 6088 SD 134 69.178 13.150 20.295 0.50 33 97 DDG	
ATOM 6089 07 101 534 68.892 13 22.968 0.50 31 30	
ATOM 6090 75 121 534 70,060 33 24,442 0.50 33 05	
ATOM 25 GYS 603 FC 22.456 25.568 0 FC	
ATOM 3002 OH2 TIP3 1 71 702 16.319 0 50	
ATOM 25 OH2 TIP3 2 25.340 2.479 1 37.82 PRT2	;
2688 OH2 TIP3 3 40.022 4.089 16 103 24.18	
2691 OH2 TIF3 4 83.745 19.577 10.510 43.09	
2694 OH2 TIPE 83.420 20 163 T-00 27.38	
ATOM 2697 OH2 TIP2 75.022 16.43e 1.00 30.85	
ATOM 2700 OV2 86.308 10 5.505 1.00 33 15	
ATOM 2703 OV3 51.888 11.346 9.284 1.00 33.55	
ATOM 2706 000 1123 8 55 125 24.141 1.00 34 30	
ATOM 2700 57 087 5.616 22.499 1.00 21 4.	
ATOM 2002 TIP3 10 52 140 4.325 32.412 1 00	
ATOM 27 OH2 TIP3 11 4.824 13.180 1 00	
ATOM 27 OH2 TIP3 12 5.600 22.910 1 00	
MTON 2718 OH2 TIP3 13 9.130 21.671 1.00 49.23	
2721 OH2 TID2 1 04.608 12.335 20 37.09	
7/.192 13 199 07 1.00 44.31	
79.201 17 295 10 1.00 32.96	
ATOM 2730 OH2 TIP2 82.988 11.608 15.77 1.00 38.51	
ATOM 2733 OK3 1/ 14.096 19.010 13.745 1.00 27.56	
ATOM 2736 000 18 38 325 0.333 1.00 23 53	
ATOM 2730 27 119 26 939 5.313 1.00 43 15	
ATOM 2749 On2 TIP3 20 34 305 5.100 1.00 30	
ATOM 2742 OH2 TIP3 21 20 300 -1.615 16.992 1 00	
Amost 2,43 OH2 TIP3 22 2.328 27 798 1 00 34.82	
NTO: 2748 OH2 TIP3 23 -11.607 38.052 1 00 45.23	
2751 OH2 TIP3 24 17.261 -6.167 1.444 1.00 43.49	
2/54 OH2 TIDE 27.724 8.124 14.00 27.13	
ATOM 2757 OH2 TERE 31.558 0 284 1.00 31.20	
ATOM 2760 OH2 mrs 26 26.907 -12 815 5.872 1.00 34.54	
ATOM 2752 On TIP3 27 28 705 12.815 28.161 1.00 48 22	
ATOM 275- 11P3 28 89 530 17.192 13.269 1 00 20	
ATOM 2766 OH2 TIP3 29 13.953 7.692 1.00	
ATOM 2769 OH2 TIP3 30 2.526 -3.576 11.086 1.00	
ATOM 2772 OH2 TIP3 31 34.919 -4.069 19.070 1.00 44.89	
2775 OH2 TIP3 32 00.124 17.865 9 324 1.00 53.72	
5.417	
SSSD/55145. v01	



	200
	-10 718 4.889 11.542 1.00 30.81
NTOM 2778 OH2 TIP3 33	-10.718 2.023 20.599 1.00 51.33
ATOM 2770 DIE	29.486
ATOM 2/01 000	6.151 0.361 1.00 48.13
ATOM 2784 OR2 7772 36	31.907
ATOM 2/6/	19.9/4 22 604 1.00 36.01
ATOM 2790 OR2 TIP3 38	61.976 23.759 1.00 20.12
ATOM 2793 UN2 TIP3 39	21.084 1.00 54.80
ATOM 2796 OH2 TIP3 40	-15.723 8.734 1.00 37.93
ATOM 2777	40.160 2.30 0.190 1.00 37.63
ATOM 2002	19.248 12.185 1.00 27.91
ATOM 2805 OH2 TTP3 43	66.836
ATOM 2000 CTD3 44	87.282 2 987 1.00 42.19
ATOM 2011 TIP3 45	74.59/ 10.582 1.00 3/.20
ATOM 2814 OH2 TIP3 46	29.192 2073 14.829 1.00 34.80
ATOM 2817 OTT TTP3 47	66.415 5510 1.00 27.42
ATOM 2020 TTD3 48	85.063 22.5 3.998 1.00 40.54
ATOM 2023 TIP3 49	-4.716 F 060 4.888 1.00 38.40
ATOM 2020 TTP3 50	19.369 5.517 24.999 1.00 29.11
ATOM 2023 TTP3 51	34.750
ATOM 2032 mrn3 52	34./40 22.80
ATOM 2000	59.994 7.505 6.080 1.00 43.73
ATOM 2000 TTP3 54	-7.401 12.004 25.108 1.00 44.32
ATOM 2012 TTP3 55	55.257 15.647 1.00 44.40
ATOM 2844 CH2 TIP3 56	68.239 0.55 18.820 1.00 29.47
ATOM 2047 TIP3 57	73.621 2304 -8.210 1.00 22.31
ATOM 2000 TIP3 58	3.399 5.505 1.00 31.02
ATOM 2855 OH2 TIP3 59	37.999 10.00 1.395 1.00 40.76
ATOM 2850 OH2 TIP3 60	29.779
ATOM 2853 OH2 TIP3 61	49.114 4 012 29.005 1.00 39.24
Alon 2005 ON2 TIP3 62	41.257
A10M 2000 ON2 TIP3 63	4 593 21.504 1.50
A10M 2000 TIP3 64	16 453 13.258 1.00
ATOM 2874 OH2 TIP3 65	4 106 3.434 1.00
ATOM 2877 OH2 TIP3 66	18 807 22.589 1.00 30 81
ATOM 2880 OH2 TIP3 67	3 666 25.021 1.00
ATOM 2883 OH2 TIP3 68	4 683 28.008 1.00
PROM 2886 OH2 TIP3 6	20.641 4.804 1.00
2889 OH2 TIP3 /	7.407 4.859 1.00
ATOM 2892 OH2 TIP3 /	1 35.007 -13.832 -2.611 1.00 33.07
NTOM 2895 OH2 1123	7 351 4.303 1.00
arou 2898 OH2 TIP3 7	32,901 2.922 13.663 1.00 39.12
ATOM 2901 OH2 TIP3	-2 666 11.033
ATOM 2904 OH2 TIPS	75 2 317 5.808 1.00
ATOM 2907 OH2 TIP3	70 27 183 3.730 0.53
ATOM 2910 OH2 TIP3	-8.812 5.887 9.703 I OD 30.79
ATOM 2913 OH2 TIP3	78 - 614 -2.195 8.694 1.00
ATOM 2916 OH2 TIP3	79 -5.304 -3.157 6.846 1.00 20.47
2919 OH2 TIP3	2.918 1.973 1.00 24.44
7 MOM 2922 OH2 TIP3	3.188 3.159 1.00 31.11
2925 OH2 TIP3	0.408 -2.516 22.270 1 00 17.62
ATOM 2928 OH2 TIP3	20.095 -6.123 -1.372 1.00 60.29
2931 OH2 TIP3	84 25.627 7.421 1.00 39.47
ATOM 2934 OH2 TIP3	85 -12.037 11.797 1.00
ATOM 2937 OH2 TIP3	86 4.000
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ATOM 2940 OVA	
ATOM TIP3 87	
NTOM -3 OH2 TIP3 88 -13 0.908 -3.278 1 00	
ATOM 2946 OH2 TTP3 00 13.493 1.004 5.310 1.00	.31
ATOM 2949 OH2 TIP3 90 15.418 -7.532 0.033 1.00 41	.13
ATOM 2952 OH2 TIP2 0: -2.128 -5.834 1.00 21	.29
ATOM 2955 OH2 TEN 12.731 4.822 1.00 57	. 55
ATOM 2959 000 69.320 27 37 4.212 1.00 44	52
ATOM 2961 072 TIP3 93 24.851 22.191 1.00 37	
ATOM 11P3 94 60 12.8/1 0.285 1.00	
ATOM 2504 Crd2 TIP3 95 10 -4.459 33.927 1 00	
OH2 TIP3 96 5.951 3.205 100	13
2970 OH2 TIP3 97 -4.233 4.430 1.00 41.	
72.950 -1 769 10 1.00 29.	לֹו
3.287 5.612 39.6	9
ATOM 2979 000 34.658 36.658 1.00 34.6	
ATOM 2992 21 221 11./17 1.00 35 4	
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ATOM 2005 OH2 TIP3 102 -13 520 -8.726 22.274 1 00 45	D <sub>.</sub>
ATOM OH2 TIP3 103 105 7.868 17 445 1	3
OH2 TIP3 104 = 10.682 =0.007	5
2994 OH2 TIP3 105 23./11 1.909 18 300 28.69	5
ATOM 2997 OH2 TIP2 -2.187 12 222 10.309 1.00 28.20	)
ATOM 3000 OH2 TIP2 100 59.483 12.399 3.320 1.00 44.98	ı
ATOM 3003 Ok2 7773 107 4.439 -70 815 33.535 1.00 39.58	
ATOM 3006 072 11P3 108 8.041 1.996 1.00 43 77	
ATOM 3000 TIP3 109 75 836 2.687 6.648 1.00 45 33	
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7 TIP3 111 15.594 14 349 1	
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3018 OH2 TIP3 112 62.927 26.453 12.807 1.00 34.21	
3021 OH2 TIP3 114 8.983 -6.631 -3.260 1.00 36.54	
3024 OH2 TIP2 8.690 4.367 1.00 47.01	
ATOM 3027 OH2 TTP2 7.941 -13 921 4.504 1.00 41.25	
ATOM 3030 ON3 TIPS 116 51.295 5.440 8.777 1.00 36.12	
ATOM 3022 077 117 20 432 10.632 1.00 38 72	
ATOM 3036 012 TIP3 118 72.882 3.7/1 15.637 1.00 31.33	
Amore 1153 [19 # 100/ 20.997 1 65	
NTON 3039 OH2 TIP3 120 33 22 711 1 20	
3042 OH2 TIP3 121 2.571 16 293 1 47.49	
UH2 TIP3 122 -12.183 7 160	
3048 OH2 TIP3 133 3.827 3.647 1.00 31.48	
7.281 7.321 2.300 46.92	
ATOM 3054 OH2 TIPS 35.682 -1.725 1.00 62.46	
ATOM 3057 OH3 T25 44.465 10.005 0.534 1.00 36.75	
ATOM 2000 11P3 126 45 247 11.089 1.00 44 75	
ATOM 3063 CH2 TIP3 127 57 386 11.893 21.405 1.00 33 51	
7 more OA2 TIP3 128	
Man 3066 OH2 TIP3 129 15.103 16.644 1 00	
3009 OH2 TIP3 130	
3072 OH2 TIP3 131 13.040 -2.760 2 176 38.13	
75.607 3 932 3 1.26	
ATOM 3078 OH2 TIPE 13.080 7 467	
ATOM 3081 ON3 1133 11.308 -9.967 2.358 1.00 35.05	
ATOM 3084 012 TIP3 134 13.716 10.995 1.00 28 96	
ATOM 3007 T1P3 135 75 400 10.170 3.848 1.00 44 5	
ATOM 3087 OH2 TIP3 136 25 Pd 3 -3.706 16.178 1.00 43	
OH2 TIP3 137 -12.949 3.950 3.950	
ATOM 3093 OH2 TIP3 138 16.285 10.803 6.585 10.803	
3096 OH2 TIP3 120 06.457 12.585 6.477 15.00 45.75	
ATOM 3099 OH2 TTD3 32.097 -4.544 0.47/ 1.00 36.37	
1123 140 44.936 7 520 2.224 1.00 28.35	
SSSD/55145. v01 7.528 11.961 1.00 46.60	

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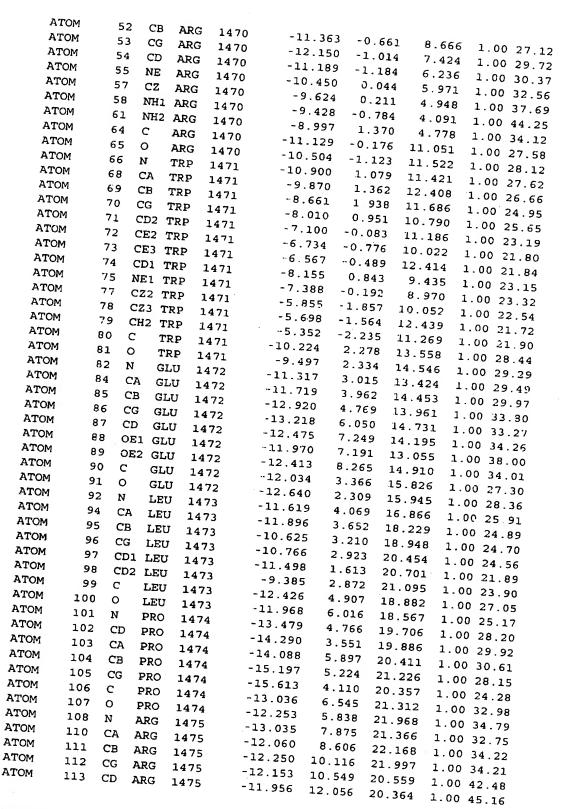
MOTA	3102	OH2	TIP3	141	80.781	12.162	16.353	1.00	41.46
ATOM	3105	OH2	TIP3	142	2.547	-7.532	-1.453	1.00	41.42
MOTA	3108	OH2	TIP3	143	31.850	-5.907	21.194	1.00	54.70
MOTA	3111	OH2	TIP3	144	74.524	-2.663	12.264	1.00	40.35
ATOM	3114	OH2	TIP3	145	7.592	6.769	-0.931	1.00	58.34
ATOM	3117	OH2	TIP3	146	71.168	5.735	21.648	1.00	27.86
MOTA	3120	OH2	TIP3	147	67.876	-4.900	8.725	1.00	33.58
MOTA	3123	OH2	TIP3	148	0.554	-10.181	6.605	1.00	75.65
ATOM	3126	OH2	TIP3	149	67.965	18.266	10.874	1.00	30.42
ATOM	3129	OH2	TIP3	150	3.509	8.125	4.021	1.00	40.77
ATOM	3132	OH2	TIP3	151	52.216	12.175	18.131	1.00	47.63
ATOM	3135	OH2	TIP3	152	-10.336	6.394	5.014	1.00	48.53
ATOM	3138	OH2	TIP3	153	76.427	1.384	-1.196	1.00	47.21
ATOM	3141	OH2	TIP3	154	10.116	-12.199	17.089	1.00	70.16
ATOM	3144	OH2	TIP3	155	34.043	14.595	18.314	1.00	40.56
AT'OM	3147	OH2	TIP3	156	2.488	8.304	16.835	1.00	64.47
ATOM	3150	OH2	TIP3	157	29.610	1.954	6.685	1.00	48.74
ATOM	3153	OH2	TIP3	158	32.578	-17.270	.12.109	1.00	37.35
ATOM	3156	OH2	TIP3	159	42.013	18.106	11.196	1.00	68.33
ATOM	3159	OH2	TIP3	160	87.646	10.346	5.465	1.00	75.39
MOTA	3162	OH2	TIP3	161	69.931	-3.739	24.921	1.00	70.42
MOTA	3165	OH2	TIP3	162	77.277	5.700	23.531	1.00	53.26
MOTA	3168	OH2	TIP3	163	34.172	15.704	1.865	1.00	44.88
ATOM	3171	OH2	TIP3	164	-9.871	7.514	7.751	1.00	39.18
ATOM	3174	OH2	TIP3	165	11.814	5.604	7.443	1.00	46.70
ATOM	3177	OH2	TIP3	166	-8.801	13.912	13.532	1.00	52.89
ATOM	3180	OH2	TIP3	167	32.195	3.409	18.336	1.00	32.33
MOTA	3183	OH2	TIP3	168	-8.858	9.696	24.279	1.00	38.90
ATOM	3186	OH2	TIP3	169	-1.135	-6.924	15.691	1.00	43.05
ATOM	3189	OH2	TIP3	170	79.806	0.323	15.371	1.00	36.91
MOTA	3192	OH2	TIP3	171	67.181	20.622	-1.545	1.00	44.72
MOTA	3195	OH2	TIP3	172	-0.823	3.732	1.065	1.00	52.11
ATOM	3198	OH2	TIP3	173	-0.130	6.021	2.491	1.00	40.87
ATOM	3201	OH2	TIP3	174	-1.027	8.941	1.064	1.00	60.72
ATOM	3204	OH2	TIP3	175	-5.566	8.867	2.163	1.00	47.25
MOTA	3207	OH2	TIP3	176	-7.259	10.294	4.033	1.00	53.61
ATOM	3210	OH2	TIP3	177	2.664	7.247	1.058	1.00	46.41
MOTA	3213	OH2	TIP3	178	5.295	10.728	8.257	1.00	39.84
MOTA	3216	OH2	TIP3	179	63.743	12.726	22.713	1.00	49.55
MOTA	3219	OH2	TIP3	180	79.165	1.016	17.948	1.00	51.41
MOTA	3222	OH2	TIP3	181	13.823	-1.538	-3.942	1.00	39.85
MOTA	3225	OH2	TIP3	182	59.255	3.213	32.873	1.00	76.77
ATOM	3228	OH2	TIP3	183	32.210	13.612	20.027	1.00	60.41
ATOM	3231	OH2	TIP3	184	72.606	16.267	22.574	1.00	60.78
ATOM	3234	OH2	TIP3	185	-0.147	5.713	30.877	1.00	50.19
MOTA	3237	OH2	TIP3	186	-1.207	-4.507	27.969	1.00	65.19
ATOM	3240	OH2	TIP3	187	81.340	15.584	16.808	1.00	64.48
MOTA	3243	OH2	TIP3	188	-17.535	3.884	23.785	1.00	57.17
MOTA	3246	OH2	TIP3	189	27.503	10.697	14.669	1.00	36.11
MOTA	3249	OH2	TIP3	190	34.585	4.535	27.618	1.00	61.68
MOTA	3252	OH2	TIP3	191	-3.701	-4.982	9.069	1.00	43.66
MOTA	3255	OH2	TIP3		42.524	7.811	22.390	1.00	34.53
ATOM	3258	OH2	TIP3		52.937	11.764	21.790	1.00	36.19
MOTA	3261	OH2	TIP3		-7.665	8.600	6.358	1.00	59.08

Amore .	
ATOM 3264 OH2 TIP3 195 86 880	
3267 OH2 TIP3 196 5.187 16.579	
ATOM 3270 OH2 TIP3 355.377 16.147 20 515	.88
ATOM 3273 OH2 TTD: 51.394 19.664 22 1.00 48	. 25
ATOM 227 1193 198 20 021 22.988 1.00 46	. 81
ATOM 3370 TIP3 199 28 950 7.226 1.00 53	98
ATOM 3200 26 522 1.019 -3.219 1.00 40	50
3282 OH2 TIP3 201 26 33 2.812 -4.295 1.00	
3285 OH2 TIP3 202 30.739 3.003 18 287	
ATOM 3288 OH2 TIP3 303 16.968 -20.752 14 310 42.	
ATOM 3291 OH2 MTD 28.177 -14 419 54.	54
ATOM 3204 11P3 204 31 489 6.134 1.00 61	
ATOM 2207 11P3 205 10 665 1.796 1.00 47	
ATOM 3205 512 11P3 206 6 926 15.731 1.00 43	
OH2 TIP3 207 12.200 6.160 1.00	12
AIOM 3303 OH2 TTP3 200 12.659 14.357 10.900 1.00 61.9	
AIOM 3306 OH2 TID 11.274 9 562 1 1.00 52.5	6
ATOM 3309 ON3 MTP3 209 11.491 12.484 1.00 48.4	
ATOM 3330 11P3 210 34 037 11.531 1.00 44 F	1
ATOM 3215 211 31.162 13.320 -1.011 1.00 48 4	
7 980 1 00	-
3318 OH2 TIP3 213 51.633 -1.971 1.00	>
3321 OH2 TIP2 224 13.599 26 FOR 49.89	
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AIOM 3327 OH2 MTD3 90.599 4 042 57.04	
ATOM 3330 11P3 216 50 139 6.342 1.00 54 00	
ATOM 3323 111 1123 217 66 523 110.526 1.00 54 64	
ATOM 3336 TIP3 218 74 880 1.024 30.536 1.00 38 41	
ATOM 11P3 219 3 222 10.591 1 00	
9.744 3.142 1.00 TIP3 220	
3342 OH2 TTP3 221 3.682 25 025 25.35	
ATOM 3345 OH2 TTP3 35.616 6.407 13 415	
ATOM 3348 OH2 TIP2 -5.381 16.006 14 17 1.00 44.48	
ATOM 3351 1.00 44 33	
ATOM 735 11P3 224 -3 701 100 53 00	,
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ATOM 7369 T1P3 226 86 344 5.0% -0.402 1.00 59 69	
3360 OH2 TIP3 227 11.220 23.133 1 00	
7.959 F CED	
ATOM 3366 OH2 TIP3 220 64.610 -8.031 20 406 1.00 63.07	
ATOM 3369 OH2 TID2 22 11.446 -17.829 12 12 48.11	
ATOM 3372 OH2 TTD 230 72.056 1 250 13.438 1.00 51.35	
ATOM 2275 11P3 231 57 350 1.830 1.00 43 80	
ATOM 3770 612 11P3 232 43 344 33 11.744 1.00 65 45	
ATOM 3303 66 733 20.728 30.066 1.00 61 53	
3381 OH2 TIP3 234 16.772 15.661 1 01.32	
22.036 4.257 1 00 13.79	
ATOM 3387 OH2 TTP3 236 12.085 2.346 27.863 1.00 61.83	
AIOM 3390 OH2 TIP2 225 04.898 -0.425 3 200 46.29	
ATOM 3393 OH2 MTD 237 72.114 28 348 3.209 1.00 50.06	
ATOM 3300 11P3 238 25 793 1.00 53 01	
ATOM 2300 OH2 TIP3 239 -18 262 27.181 1.00 55 10	
3399 OH2 TIP3 240 10.614 12.607 1 00	
3402 OH2 TIP3 241	
ATOM 3405 OH2 TIP3 242 22.712 -15.818 -2 236 46.53	
AIOM 3408 OH2 MTD 29.700 9.495 10 1.00 47.29	
ATOM 2412 11193 243 63 207 18.074 1.00 40 10	
ATOM 344 61 450 5.497 1.00 49 00	
ATOM 241 OH2 TIP3 245 -0 217 /.093 11.497 1.00 45 71	
341/ OH2 TIP3 246 66 196 2.232 32.172 1.00 46 12	
6.250 12 150	
12.139 1.00 34.47	



TABLE 3

Atom		Atom	A.A		x	Y	$\mathbf{z}$	occ	, <b>B</b>	
No.		Гуре	Тур	e No.						
MOTA	1	N	GLU	1464	-13.712	16.996	8.424	1.00	61.15	
MOTA	. 3	CA	GLU	1464	-12.478	17.133	7.646	1.00	60.03	
MOTA	4	CB	GLU	1464	-11.465	18.020	8.378	1.00	62.43	
ATOM	5	C	GLU	1464	-11.865	15.766	7.319	1.00	57.36	
MOTA	6	0	GLU	1464	-11.765	15.402	6.145	1.00	60.80	
ATOM	7	N	LEU	1465	-11.466	15.003	8.333	1.00	50.25	
MOTA	9	CA	LEU	1465	-10.899	13.691	8.067	1.00	42.73	
MOTA	10	CB	LEU	1465	-10.097	13.171	9.258	1.00	41.34	
ATOM	11	CG	LEU	1465	-8.571	13.277	9.169	1.00	39.78	
ATOM	12		LEU	1465	-8.175	14.728	8.977	1.00	45.14	
ATOM	13	CD2	LEU	1465	-7.926	12.722	10.426	1.00	34.20	-
ATOM	14	С	LEU	1465	-12.009	12.706	7.748	1.00	39.42	
MOTA	15	0	LEU	1465	-13.070	12.719	8.375	1.00	36.63	
ATOM	1.6	N	PRO	1466	.11.821	11.919	6.682	1.00	38.54	
ATOM	17	CD	PRO	1466	-10.682	12.019	5.751	1.00	37.04	
ATOM	18	CA	PRO	1466	-12.781	10.902	6.232	1.00	38.75	
ATOM	1.9	CB	PRO	1466	-12.176	10.426	4.910	1.00	39.49	
ATOM	20	CG	PRO	1466	-10.681	10.667	5.109	1.00	40.64	
ATOM	21	C	PRO	1466	-12.859	9.756	7.246	1.00	39.08	
MOTA	22	0	PRO	1466	-11.834	9.283	7.748	1.00	41.23	
MOTA	23	N	GLU	1467	-14.064	9.278	7.513	1.00	37.11	
. ATOM	25	CA	GľŪ	1467	-14.247	8.213	8.482	1.00	35.96	
MOTA	26	CB	GLU	1467	-15.725	8.123	8.863	1.00	39.90	
ATOM	27	CG	GLU	1467	-16.334	9.410	9.417	1.00	46.64	
MOTA	28	CD	GLU	1467	-17.823	9.280	9.694	1.00	51.50	
MOTA	29	OE1	GLU	1467	-18.294	8.135	9.854	1.00	54.17	
ATOM	30	OE2	GLU	1467	-18.529	10.315	9.756	1.00	53.39	
ATOM	31	С	GLU	1467	-13.794	6.865	7.939	1.00	33.77	
MOTA	32	0	GLU	1467	-13.885	6.632	6.740	1.00	36.27	
MOTA	33	N	ASP	1468	-13.291	5.991	8.813	1.00	29.80	
MOTA	35	CA	ASP	1468	-12.869	4.649	8.409	1.00	28.19	
ATOM	36	CB	ASP	1468	-11.362	4.567	8.120	1.00	27.83	
MOTA	37	CG	ASP	1468	-10.942	3.223	7.507	1.00	27.78	
ATOM	38	OD1	ASP	1468	-11.689	2.225	7.592	1.00	25.64	
ATOM	39	OD2	ASP	1468	-9.836	3.165	6.935	1.00	27.59	
ATOM	40	C	ASP	1468	-13.244	3.672	9.512	1.00	28.05	
ATOM	41	0	ASP	1468	-12.462	3.404	10.437	1.00	25.89	
ATOM	42	N	PRO	1469	-14.446	3.089	9.403	1.00	29.07	
ATOM	43	CD	PRO	1469	-15.401	3.311	8.298	1.00	29.93	
MOTA	44	CA	PRO	1469	-14.981	2.124	10.365	1.00		
MOTA	45	CB	PRO	1469	-16.235	1.615	9.659	1.00	30.89	
MOTA	46	CG	PRO	1469	-16.690	2.811	8.879	1.00		
MOTA	47	С	PRO	1469	-14.029	0.974	10.687	1.00		
MOTA	48	0	PRO	1469	-14.136	0.364	11.748	1.00		
ATOM	49	N	ARG	1470	-13.128	0.666	9.758	1.00		
ATOM	51	CA	ARG	1470	-12.161	-0.414	9.947	1.00		
				-	<b></b>				_0.04	



MOTA	114	NE	ARG	1475	-11.655	12.317	18.954	1.00 45.65
ATOM	116	CZ	ARG	1475	-10.447	12.599	18.484	1.00 41.31
ATOM	117	NH1	ARG	1475	-9.420	12.686	19.318	1.00 35.94
ATOM	120	NH2	ARG	1475	-10.253	12.673	17.172	1.00 42.37
ATOM	123	C	ARG	1475	-12.114	8.232	23.641	1.00 35.29
MOTA	124	0	ARG	1475	-11.094	8.178	24.318	1.00 37.28
ATOM	125	N	ASP	1476	-13.304	7.931	24.129	1.00 35.37
ATOM	127	CA	ASP	1476	-13.468	7.570	25.526	1.00 36.97
MOTA	128	CB	ASP	1476	-14.952	7.586	25.896	1.00 39.47
ATOM	129	CG	ASP	1476	-15.748	6.501	25.205	1.00 40.02
ATOM	130	OD1	ASP	1476	-15.221	5.809	24.320	1.00 41.08
MOTA	131	OD2	ASP	1476	-16.926	6.327	25.571	1.00 47.00
ATOM	132	С	ASP	1476	-12.850	6.225	25.894	1.00 36.07
MOTA	133	0	ASP	1476	-12 830	5.842	27.066	1.00 36.26
ATOM	134	N	ARG	1477	-12.382	5.495	24.888	1.00 36.94
ATOM	136	CA	ARG	1477	-11.766	4.189	25.104	1.00 35.22
ATOM	137	CB	ARG	1477	-12.081	3.268	23.925	1.00 34.29
ATOM	138	CG	ARG	1477	-13.546	3.056	23.675	1.00 32.23
ATOM	139	CD	ARG	1477	-14.206	2.434	24.879	1.00 30.56
ATOM	140	NE	ARG	1477	-14.426	3.419	25.925	1.00 31.86
ATOM	142	CZ	ARG	1477	-14.730	3.126	27.182	1.00 33.09
ATOM	1.43	NH1	ARG	1477	-14.855	1.858	27.563	1.00 35.00
ATOM	146	NH2	ARG	1477	-14.904	4.101	28.053	1.00 29.62
ATOM	149	C	ARG	1477	-10.262	4.270	25.271	1.00 35.51
ATOM	1.50	0	ARG	1477	-9.621	3.290	25.637	1.00 35.44
ATOM	151	N	LEU	1478	-9.704	5.444	25.023	1.00 34.59
ATOM	i53	CA	LEU	1478	-8.270	5.630	25.129	1.00 36.35
ATOM	154	CB	LEU	1.478	-7.750	6.254	23.840	1.00 36.41
ATOM	155	CG	LEU	1478	-6.250	6.185	23.55€	1.00 37.19
MOTA	156	CD1	LEU	1478	-5.791	4.728	23.479	1.00 34.63
MOTA	157	CD2	LEU	1478	-5.959	6.914	22.251	1 00 34.88
ATOM	158	C	LEU	1478	-7.901	6.517	26.325	1.00 38.74
ATOM	159	0	LEU	1478	-8.146	7.733	26.309	1.00 41.20
ATOM	160	N	VAL	1479	-7.311	5.907	27.355	1.00 36.92
ATOM	162	CA	VAL	1479	-6.885	6.622	28.560	1.00 35.79
ATOM	163	СВ	VAL	1479	-6.929	5.693	29.780	1.60 35.81
ATOM	164	CG1	VAL	1479	-6.579	6.453	31.032	1.00 40.11
ATOM	165	CG2	VAL	1479	-8.302	5.056	29.907	1.00 35.59
MOTA	166	С	VAL	1479	-5.438	7.118	28.362	1.00 36.60
ATOM	167	0	VAL	1479	-4.479	6.369	28.583	1.00 33.48
ATOM	168	N	LEU	1480	-5.282	8.372	27.938	1.00 39.09
ATOM	170	CA	LEU	1480	-3.949	8.932	27.675	1.00 42.05
ATOM	171	CB	LEU	1480	-4.040	10.277	26.952 <sup>-</sup>	1.00 41.08
ATOM	172	CG	LEU	1480	-4.633	10.286	25.529	1.00 39.28
ATOM	173	CD1		1480	-4.766	11.720	25.051	1.00 40.04
ATOM	174	CD2		1480	-3.758	9.489	24.582	1.00 39.66
ATOM	175	С	LEU	1480	-3.001	9.027	28.867	1.00 41.51
ATOM	176	0	LEU	1480	-3.312	9.637	29.886	1.00 41.73
ATOM	177	N	GLY	1481	-1.817	8.444	28.697	1.00 40.68
ATOM	179	CA	GLY	1481	-0.849	8.439	29.775	1.00 41.28
ATOM	180	С	GLY	1481	0.412	9.225	29.529	1.00 43.08
ATOM	181	0	GLY	1481	0.474	10.147	28.701	1.00 45.65
				_	<del>-</del>			

ת	OM					
		182		LYS	1482	2 1 401
	OM	184	CA	LYS	1482	8.825 30.219 1 00 43 54
	OM	185	CB	LYS	1482	2.781 9.453 30.128 1.00 42.74
AT		186	CG	LYS	1482	3.670 8 842 31 220 1 25
AT		187	CD	LYS	1482	3.155 8.979 30 954 3 4
ATO		188	CE	LYS	1482	3.867 7.716 31 392 1 32
ATO	MC	189	NZ	LYS		5.373 6.518 30 507 3 56.63
ATC	MC	193	C	LYS	1482	6.199
ATC	M	194	0		1482	3.552 9.433 1.00 59.97
ATO	M	195	N	LYS	1482	3.557
ATO		196		PRO	1483	4.259 10 521 28.111 1.00 44.68
ATO		197	CD	PRO	1483	4.339 17 700 20.481 1.00 44.06
ATO		198	CA	PRO	1483	5.005 10 573 29.208 1.00 43.53
ATO					1483	5 500 20.3/3 2/.208 1.00 44 00
ATOM		199		PRO	1483	4 630 27.281 1.00 43 17
ATON	_	200		PRO	1483	6 172 28.114 1.00 43 75
ATOM	•	201		PRO :	1483	6 052 27 116 1.00 43 47
ATOM		202	N j		1484	28.120 1 00 43 76
		204	CA I		1484	25.932 1 00 41 21
ATOM		205	CB [		484	8.045 25.663 1 00 38 05
ATOM	•	06	CG L		484	6.803 24.927 1 00 33 30
ATOM		07	CD1 L	EU 1	484	5.001 5.992 25.770 1 00 21 00
ATOM	~	80	CD2 L		464	3.258 4.914 24.975 1 CO 27 47
ATOM		09 !	_		484	5.396 26 952 1 42
MOTA	2.	10 (	_		184 484	0.603 8.710 24 per
ATOM	2:	11 1			185	0.334 9.499 23 960 1 00
ATOM	2.	13 (				9.843 8.387 25 197 1
ATOM	23				185	8,923 24 512
ATOM	21				185	11.261 10.408 24 697 1 00 50.32
ATOM	21				85	11.036 10.973 25 770
ATOM	21			<b></b>	86 .	11.747 11.072 23.647
ATOM	21	_				12.081 12.402
ATOM	22					13.489 13 545
ATOM	22	_	GL			12.014 12.102
ATOM	22	-	GLI			12.901 13.070
ATOM	224					10.975 12 202 21.949 1.00 64.10
ATOM	225	_				10.792 13 532 21.319 1.00 62.29
ATOM	226	_	GLY		37	11.469 13 001
ATOM			GLY		7	11.447 13 425
ATOM	227 229		ALA			12.073 17 774
ATOM						12 721 13 214 19.239 1.00 57.19
ATOM	230		ALA	148	8	13.477 9 504 18.140 1.00 55.59
ATOM	231		ALA	148	8	13 500 18.663 1.00 56 35
ATOM	232	0	ALA	148	8	17.112 1.00 54 96
ATOM	233	N	PHE	1489	9	10.500 15.913 1.00 56 42
	235	CA	PHE	1489		9 403 10.241 17.598 1.00 54 99
ATOM	236	CB	PHE	1489	)	9 057 16.721 1.00 54 07
ATOM	237	CG	PHE	1489		8.454 17.162 1 00 51 10
ATOM	238	CD1	PHE	1489		7.373 17.137 1 00 46 22
ATOM	239	CD2	PHE	1489		7.093 18.271 1 00 46 03
MOTA	240	CE1	PHE	1489		6.612 15.984 1 00 40 32
ATOM	241	CE2	PHE	1489		11.385 6.090 18.262 1 00 47 41
ATOM	242	CZ	PHE	1489		11.040 5.601 15.003
ATOM	243	C	PHE			11.794 5.336 17.111 1.00 48.23
				1489		8.261 10 51
CCCD /== -						10.814 16.748 1.00 54.90

ATOM	244	0	PHE	1489	7.199	10.565	16.184	1.00	59.10
MOTA	245	N	GLY	1490	8.431	11.908	17.504		53.55
ATOM	247	CA	GLY	1490	7.432	12.958	17.611	1.00	50.20
ATOM	248	С	GLY	1490	6.745	12.844	18.942	1.00	49.82
ATOM .	249	0	GLY	1490	7.266	12.161	19.837	1.00	50.95
MOTA	250	N	GLN	1491	5.614	13.514	19.124	1.00	49.53
ATOM	252	CA	GLN	1491	4.922	13.441	20.395	1.00	49.16
ATOM	253	CB	GLN	1491	3.927	14.590	20.564	1.00	51.74
ATOM	254	CG	GLN	1491	3.439	14.796	21.994	1.00	64.00
MOTA	255	CD	GLN	1491	2.545	16.039	22.180	1.00	71.35
MOTA	256	OE1		1491	2.534	16.922	21.352	1.00	77.94
ATOM	257	NE2		1491	1.824	16.083	23.289	1.00	76.51
ATOM	260	C	GLN	1491	4.207	12.083	20.505		45.94
ATOM	261	0	GLN	1491	. 3.151.	11.869	19.919	1.00	48.02
MOTA	262	N	VAL	1492	4.848	11.129	21.184	1.00	41.00
ATOM	264	CA	VAL	1492	4.293	9.810	21.421	1.00	37.44
ATOM	265	CB	VAL	1492	5.235	8.665	21.025	1.00	34.74
MOTA	266	CG1	VAL	1492	4.593	7.325	21.285	1.00	28.97
ATOM	267	CG2	VAL	1492	5.632	8.769	19.553	1.00	35.78
MOTA	268	C	VAL	1492	4.014	9.621	22.901	1.00	38.67
ATOM	269	0	VAL	1492	4.907	9.769	23.735	1.00	38.62
ATOM	270	И	VAL	1493	2.776	9.276	23.250	1.00	39.98
MOTA	272	CA	VAL	1.493	2.423	9.062	24.653	1.00	37.79
MOTA	273	CB	LAV	1493	1.257	9.970	25.093	1.00	37.36
MOTA	274	CG1	VAL	1493	1.489	11.403	24.689	1.00	39.11
ATOM	275	CG2	VAL	1493	-0.074	9.480	24.555	1.00	38.99
MOTA	276	С	VAL	1493	2.052	7.603	24.877	1.00	36.38
ATOM	277	0	VAL	1493	1.759	6.874	23.945	1.00	37.73
MOTA	278	N	LEU	1494	2.094	7.176	26.123	1.00	35.42
ATOM	280	CA	LEU	1494	1.718	5.817	26.483	1.00	33.65
ATOM	281	CB	LEU	1494	2.536	5.291	27.670		29.88
ATOM	282	CG	LEU	1494	2.117	3.945	28.279	1.00	30.31
MOTA	283	CD1	LEU	1494	2.103	2.844	27.244	1.00	30.83
MOTA	284	CD2	LEU	1494	3.049	3.574	29.400	1.00	32.12
MOTA	285	C	LEU	1494	0.260	5.934	26.870	1.00	34.27
ATOM	286	0	LEU	1494	-0.168	6.994	27.348	1.00	34.85
MOTA	287	N	ALA	1495	-0.527	4.898	26.608	1.00	32.20
MOTA	289	CA	ALA	1495	-1.930	4.954	26.980	1.00	29.71
ATOM	290	CB	ALA	1495	-2.724	5.722	25.930	1.00	25.48
ATOM	291	С	ALA	1495	-2.499	3.567	27.183		28.85
MOTA	292	0	ALA	1495	-1.826	2.563	26.998	1.00	27.28
ATOM	293	N	GLU	1496	-3.743	3.519	27.615	1.00	32.20
ATOM	295	CA	GLU	1496	-4.413	2.250	27.824		33.34
ATOM	296	CB	GLU	1496	-4.735	2.063	29.301	1.00	35.65
ATOM	297	CG	GLU	1496	-3.521	1.962	30.198	1.00	39.14
ATOM	298	CD	GLU	1496	-3.899	2.045	31.663	1.00	42.57
MOTA	299		GLU	1496	-4.469	3.083	32.061		42.59
ATOM	300		GLU	1496	-3.646	1.069	32.407	1.00	42.76
ATOM	301	С	GLU	1496	-5.692	2.274	26.994	1.00	33.40
ATOM	302	0	GLU	1496	-6.439	3.261	27.017	1.00	34.36
MOTA	303	N	ALA	1497	-5.875	1.247	26.177	1.00	31.67
ATOM	305	CA	ALA	1497	-7.051	1.168	25.351	1.00	31.23

	rom 3	6 CB	ALA 149	7
	OM 30	7 C	ALA 149	0.750 23 952 4
	'OM 30	8 0	ALA 149	0.168 25 074
AT		9 N	ILE 149	7 -7.599 -0.954 26 261
AT		l CA	ILE 149	-9.218 0.602 26 202
ATO				-10.222 -0.294 36 054
ATO	OM 31			-11.294 0.453 27.670
ATO				-12.267 -0.551 29 300
ATC	OM 315			-10.663 1.316 28 270
ATO	)M 316	_	~-20	-11.656
ATO				-10.953 -0.000 23.419 1.00 31.69
ATO	M 318		ILE 1498	-11.571 -0.327
ATO	M 320		GLY 1499	-10.859 -2.245 24.0// 1.00 37.46
ATO			GLY 1499	-11.544 -2 010 23.339 1.00 43.14
ATON		_	GLY 1499	-10.673 -3.200 1.00 46.90
ATOM			LY 1499	-9.921 -4.369
ATOM			EU 1500	-10.739 -2.500 -3.387 1.00 51.47
ATOM		_	EU 1500	-10 002 - 22.223 1.00 49 92
ATOM			EU 1500	-8 470 - 20.973 1.00 49 62
ATOM	·		EU 1500	7 504 21.185 1.00 49 96
ATOM		CD1 L	EU 1500	-6 060 - 21.167 1.00 49 26
ATOM		CD2 L		-7 520 2.21/ 21.284 1.00 47 17
ATOM	330		EU 1500	-10 525 V.003 19.899 1.00 47 80
ATOM	331		EU 1500	-10 400 - 20.275 1.00 49 49
ATOM	332	N PI	RO 1505	-13 252 - 20.806 1.00 47 99
ATOM	333	CD PF	O 1505	-13 077 - 25.284 1.00 50.58
ATOM	334	CA PR	~~~	-14 107 11/3 25.239 1.00 51 43
ATOM	335	CB PR	0 1505	-15 540 - 25.779 1.00 48 GR
ATOM		CG PR	0 1505	-15 216 25.627 1.00 48 59
ATOM		C PR	0 1505	-13 004 25.940 1.00 51 66
ATOM		) PR	1505	-13 003 27.227 1.00 44 50
ATOM	3.4-	N ASI	<b>1</b> 1506	-13 640 - 202 27.531 1.00 42 72
ATOM		CA ASI	1506	-13 222 - 28.102 1.00 42 10
ATOM		B ASN	1506	~14 202 - 29.497 1.00 45 05
ATOM		G ASN		215 652 30.434 1.00 47 04
ATOM	344 C	D1 ASN	1506	-15 000 3.433 30.395 1.00 48 72
ATOM		D2 ASN	1506	30,487 1 00 50
ATOM	348 C	ASN		30.260 1 00 53 15
ATOM	349 O	ASN	1506	49.836 1 nn 4c m
ATOM	350 N	ARG	1507	31.008 1 00 46 55
ATOM	352 C	ARG	1507	28.806 1 00 1-
	353 CI	ARG	1507	28.976 1 00 47 77
ATOM	354 CC	ARG	1507	-6.650 28.142 1.00 54
ATOM	355 CI	ARG	1507	-9.327 -7.993 28.781 7 00 64 50
ATOM	356 NE		1507	-8.180 29.963 1 00 71
ATOM	358 CZ		1507	-0.592 -9.494 30.556 1 00 75
ATOM		1 ARG	1507	-0.030 -9.898 31.689 1.00.03.54
ATOM	362 NH	2 ARG	1507	-7.219 -9.096 32.375 1.00 81.64
ATOM	365 C	ARG		-8.340 -11.093 32 174
ATOM	366 O	ARG	1507 1507	-8.871 -4.234 28 485
ATOM	367 N	VAL		-9.227 -3.695 27 440
ATOM	369 CA	VAL	1508	-7.912 -3.749 29 265
70000	370 CB	VAL	1508	-7.143 -2.598 28 830 1.00 40.84
	-2	AUTI	1508	-6.786 -1 604
				29.961 1.00 34.90

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ATOM	371	CG1	VAL	1508	-8.038	-1.124	30.646	1.00 41.81
ATOM	372	CG2		1508	-5.850	-2.226	30.944	1.00 35.89
ATOM	373	C	VAL	1508	-5.874	-3.147	28.211	1.00 36.81
ATOM	374	0	VAL	1508	-5.371	-4.191	28.637	1.00 35.13
ATOM	375	N	THR	1509	-5.393	-2.465	27.180	1.00 36.04
MOTA	377	CA	THR	1509	-4.184	-2.854	26.485	1.00 33.31
ATOM	378	CB	THR	1509	-4.503	-3.254	25.025	1.00 33.79
ATOM	379	OG1	THR	1509	-5.511	-4.275	25.014	1.00 33.98
ATOM	381	CG2	THR	1509	-3.259	-3.774	24.321	1.00 32.78
ATOM	382	С	THR	1509	-3.268	-1.627	26.453	1.00 32.37
ATOM	383	0	THR	1509	-3.718	-0.533	26.113	1.00 31.97
ATOM	384	N	LYS	1510	-2.015	-1.786	26.884	1.00 32.96
ATOM	386	CA	LYS	1510	-1.071	-0.673	26.828	1.00 33.25
ATOM	387	CB	LYS	1510	0.157	-0.902	27.699	1.00 34.65
ATOM	388	CG	LYS	1510	-0.093	-0.909	29.197	1.00 39.64
ATOM	389	CD	LYS	1510	1.237	-1.105	29.913	1.00 43.51
ATOM	390	CE	LYS	1510	1.110	-1.949	31.173	1.00 48.42
ATOM	391	NZ	LYS	1510	0.399	-1.256	32.287	1.00 53.03
ATOM	395	C	LYS	1510	-0.646	-0.550	25.370	1.00 32.26
ATOM	396	0	LYS	1510	-0.240	-1.533	24.736	1.00 30.20
ATOM	397	N	VAL	1511	-0.760	0.665	24.849	1.00 32.28
ATOM	399	CA	VAL	1511	.0.436	0.980	23.472	1.00 30.73
ATOM	400	CB	VAL	1511	-1.738	1.140	22.666	1.00 32.25
ATOM	401	CG1	VAL	1511		-0.147	22.723	1.00 29.00
MOTA	402	CG2	VAL	1511	-2.549	2,347	23.193	1.00 29.17
ATOM	403	С	VAL	1511	0.329	2.307	23.423	1.00 30.91
ATOM	404	0	VAL	1511	0.445	3.008	24.433	1.00 31.94
ATOM	405	И	ALA	1512	0.842	2.658	22.250	1.00 27.30
ATOM	407	CA	ALA	1512	1.550	3.914	22.094	1.00 24.22
ATOM	408	CB	ALA	1512	2.921	3.694	21.493	1.00 23.39
MOTA	409	С	ALA	1512	0.698	4.769	21.181	1.00 23.62
ATOM	410	0	ALA	1512	0.116	4.271	20.228	1.00 22.69
ATOM	411	N	VAL	1513	0.605	6.054	21.484	1.00 27.51
ATOM	413	CA	VAL	1513	-0.192	6.984	20.688	1.00 30.03
MOTA	414	CB	VAL	1513	-1.359	7.613	21.522	1.00 28.31
ATOM	415		VAL	1513	-2.218	8.522	20.650	1.00 28.93
ATOM	416		VAL	1513	-2.214	6.542	22.159	1.00 26.00
ATOM	417	C	VAL	1513	0.674	8.108	20.107	1.00 31.21
ATOM	418	0	VAL	1513	1.370	8.816	20.834	1.00 29.73
ATOM	419	N	LYS	1514	0.631	8.225	18.784	1.00 33.99
ATOM.	421	CA	LYS	1514	1.342	9.258	18.037	1.00 35.44
ATOM	422	СВ	LYS	1514	1.831	8.692	16.707	1.00 34.55
ATOM	423	CG	LYS	1514	2.835	7.586	16.872	1.00 35.38
ATOM	424	CD	LYS	1514	3.025	6.807	15.599	1.00 36.87
ATOM	425	CE	LYS	1514	3.457	7.710	14.438	1.00 45.19
ATOM	426	NZ	LYS	1514	4.598	8.622	14.755	1.00 44.31
ATOM	430	C	LYS	1514	0.304	10.345	17.761	1.00 35.97
ATOM	431	0	LYS	1514	-0.806	10.343	17.761	1.00 34.39
ATOM	432	N	MET	1515	0.673	11.596	18.028	1.00 34.39
ATOM	434	CA	MET	1515	-0.207		17.835	1.00 38.17
ATOM	434	CB	MET			12.747		
				1515	-0.901	13.098	19.145	1.00 39.54
ATOM	436	CG	MET	1515	0.075	13.428	20.255	1.00 39.11

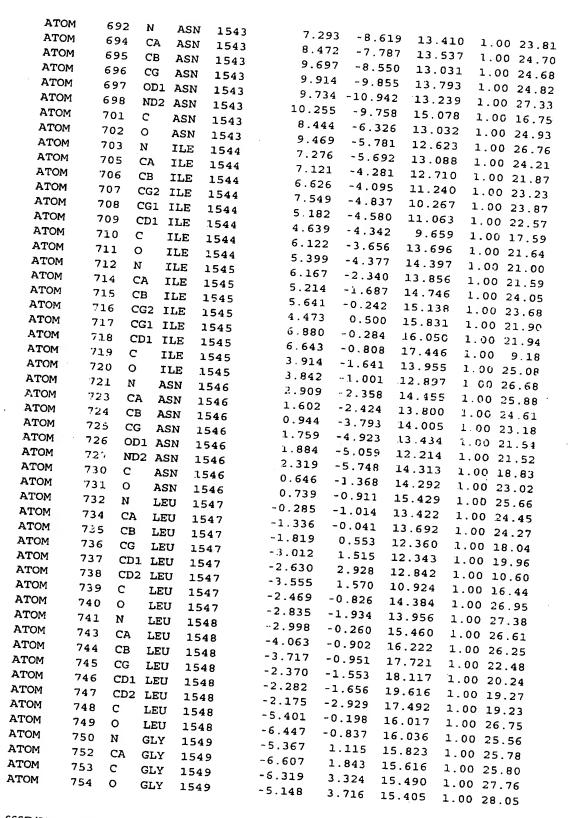
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ATOM 439 C MET 1515 -0.766 13.612 21.799 1.00 43.85 ATOM 439 C MET 1515 -0.212 11.937 22.087 1.00 46.18 ATOM 440 0 MET 1515 0.612 13.939 17.345 1.00 45.72 ATOM 441 N LEU 1516 -0.053 14.962 16.872 1.00 48.73 ATOM 444 CB LEU 1516 -0.053 14.962 16.872 1.00 48.73 ATOM 445 CG LEU 1516 -0.152 16.917 15.374 1.00 49.77 ATOM 446 CD1 LEU 1516 -0.413 16.254 14.036 1.00 49.77 ATOM 447 CD2 LEU 1516 -0.413 16.254 14.036 1.00 49.77 ATOM 449 O LEU 1516 -0.884 16.102 13.285 1.00 48.04 ATOM 449 N LEU 1516 -0.810 17.119 17.651 1.00 42.80 ATOM 450 N LYS 1517 1.580 18.174 17.402 1.00 60.97 ATOM 451 CB LYS 1517 1.823 19.193 18.416 1.00 65.19 ATOM 452 CR LYS 1517 1.823 19.193 18.416 1.00 65.19 ATOM 455 CD LYS 1517 1.024 18.559 18.529 1.00 72.86 ATOM 465 C LYS 1517 5.646 18.935 17.022 1.00 69.34 ATOM 456 C LYS 1517 6.686 17.851 18.197 1.00 75.45 ATOM 466 C LYS 1518 -0.010 18.214 17.649 1.00 75.45 ATOM 466 C SER 1518 -0.002 23.322 20.202 1.00 68.20 ATOM 467 C SER 1518 -0.002 23.322 20.202 1.00 68.99 ATOM 470 C SER 1518 -0.002 23.322 20.202 1.00 68.99 ATOM 471 CA ASP 1519 1.179 22.492 11.00 77.59 ATOM 472 CB ASP 1519 1.179 22.492 11.00 77.59 ATOM 473 C ASP 1519 1.179 22.492 11.00 77.59 ATOM 474 C ASP 1519 1.179 22.492 1.00 77.59 ATOM 475 N ASP 1519 1.179 22.492 11.00 77.59 ATOM 470 C ASP 1519 1.179 22.493 17.006 1.00 77.59 ATOM 472 C BAP 1519 1.1799 22.285 12.799 1.00 77.59 ATOM 473 C ASP 1519 1.199 22.852 1.00 77.59 ATOM 474 C ASP 1519 1.199 22.852 12.799 1.00 77.59 ATOM 475 N ALA 1520 1.466 22.265 11.401 1.00 69.75 ATOM 485 CG LYS 1521 1.950 23.310 9.727 1.00 77.44 ATOM 485 CG LYS 1517 0.889 22.653 11.00 77.59 ATOM 478 CB ALA 1520 0.898 22.553 11.00 77.59 ATOM 485 CG LYS 1521 1.950 23.310 9.727 1.00 77.49 ATOM 486 C THR 1521 1.950 23.310 9.792 1.00 77.147 ATOM 487 CG2 LYS 1521 1.950 23.310 9.792 1.00 77.59 ATOM 488 C THR 1521 1.950 23.310 9.793 1.00 66.50 ATOM 499 CB LYS 1523 1.125 18.878 7.006 6.870 1.00 66.75 ATOM 490 CB LYS 1523 1.125 18.878 7.006 6.610 1.00 66.75 ATOM 496 CB LYS 1523 1.125 18.878 7.006 6.620 1.00 66.57		
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ATOM 449 C LEU 1516 ATOM 444 C B LEU 1516 ATOM 445 CB LEU 1516 ATOM 447 CD LEU 1516 ATOM 448 C LEU 1516 ATOM 449 C LEU 1516 ATOM 449 CB LEU 1516 ATOM 440 CB LEU 1516 ATOM 445 CB LEU 1516 ATOM 445 CB LEU 1516 ATOM 446 CB LEU 1516 ATOM 447 CD LEU 1516 ATOM 448 C LEU 1516 ATOM 449 C LEU 1516 ATOM 449 CB LEU 1516 ATOM 440 CB LEU 1516 ATOM 450 CB LEU 1516 ATOM 460 CB LEU 160 C	ATOM 438 CF MET	0.766 13 612 25 5
ATOM 440 0 MET 1515 ATOM 441 N LEU 1516 ATOM 441 N LEU 1516 ATOM 444 CA LEU 1516 ATOM 444 CB LEU 1516 ATOM 445 CG LEU 1516 ATOM 446 CD1 LEU 1516 ATOM 447 CD2 LEU 1516 ATOM 448 C LEU 1516 ATOM 449 O LEU 1516 ATOM 450 O LEU 1516 ATOM 451 CB LYS 1517 ATOM 452 CA LYS 1517 ATOM 452 CA LYS 1517 ATOM 455 CD LYS 1517 ATOM 456 CB LYS 1517 ATOM 456 CB LYS 1517 ATOM 457 NZ LYS 1517 ATOM 466 CB SER 1518 ATOM 467 C SER 1518 ATOM 467 C SER 1518 ATOM 468 O SER 1518 ATOM 467 C SER 1518 ATOM 471 CA ASP 1519 ATOM 472 CB ASP 1519 ATOM 473 C ASP 1519 ATOM 473 C ASP 1519 ATOM 474 C ASP 1519 ATOM 475 N ALA 1520 ATOM 476 C SER 1518 ATOM 476 C SER 1518 ATOM 477 CA ASP 1519 ATOM 478 CB ALA 1520 ATOM 479 C ALA 1520 ATOM 479 C ALA 1520 ATOM 488 CB THR 1521 ATOM 489 CB LYS 1521 ATOM 489 CB LYS 1522 ATOM 489 CB LYS 1523 ATOM 499 CB LYS 1520 ATOM 499 CB LYS 1523	ATOM 439 C MID	5 -1 212 25 21.799 1.00 42 05
ATOM 441 N LEU 1516 -0.053 14.962 17.45 1.00 43.73 ATOM 444 CB LEU 1516 -0.053 14.962 16.872 1.00 48.73 ATOM 444 CB LEU 1516 -0.640 16.175 16.482 1.00 48.73 ATOM 445 CG LEU 1516 -0.152 16.917 15.374 1.00 49.77 ATOM 447 CD2 LEU 1516 -0.413 16.254 14.036 1.00 49.77 ATOM 448 CD1 LEU 1516 -0.413 16.254 14.036 1.00 48.16 ATOM 449 CD2 LEU 1516 -0.884 16.102 13.285 1.00 48.16 ATOM 449 O LEU 1516 -0.884 16.102 13.285 1.00 48.16 ATOM 450 N LYS 1517 -0.217 16.927 18.703 1.00 55.67 ATOM 452 CA LYS 1517 1.823 19.193 18.415 1.00 65.19 ATOM 453 CB LYS 1517 1.823 19.193 18.416 1.00 69.13 ATOM 455 CD LYS 1517 1.823 19.193 18.416 1.00 69.13 ATOM 456 CD LYS 1517 4.294 18.559 18.525 1.00 74.98 ATOM 466 CD LYS 1517 5.646 18.95 17.929 1.00 74.98 ATOM 467 C LYS 1517 8.010 18.241 17.649 1.00 79.78 ATOM 468 CD LYS 1518 -0.00 18.241 17.649 1.00 79.78 ATOM 468 CD LYS 1518 -0.00 18.241 17.649 1.00 75.45 ATOM 467 C SER 1518 -0.107 22.422 18.972 1.00 74.98 ATOM 468 CB SER 1518 -0.107 22.422 18.972 1.00 74.98 ATOM 468 CB SER 1518 -0.107 23.322 20.202 1.00 69.89 ATOM 468 CB SER 1518 -0.107 23.302 20.421 17.006 1.59 ATOM 471 CA ASP 1519 1.912 23.525 1.959 1.00 77.59 ATOM 473 C ASP 1519 1.912 23.525 1.959 1.00 77.59 ATOM 473 C ASP 1519 1.912 23.525 1.959 1.00 77.59 ATOM 474 CB ALA 1520 1.468 22.265 1.4958 1.00 77.59 ATOM 479 C ALA 1520 1.504 22.858 12.797 1.00 77.59 ATOM 480 C ALA 1520 1.504 22.858 12.797 1.00 70.21 ATOM 480 C ALA 1520 1.504 22.858 12.797 1.00 70.21 ATOM 480 C ALA 1520 1.504 22.858 12.797 1.00 70.21 ATOM 480 C ALA 1520 1.504 22.858 12.797 1.00 70.21 ATOM 480 C ALA 1520 1.689 22.653 10.034 1.00 71.01 ATOM 480 C ALA 1520 1.504 22.858 12.797 1.00 70.21 ATOM 480 C ALA 1520 1.689 22.653 10.034 1.00 71.01 ATOM 480 C ALA 1520 1.689 22.653 10.034 1.00 71.01 ATOM 480 C ALA 1520 1.689 22.653 10.034 1.00 70.01 ATOM 480 C ALA 1520 1.699 22.159 9.922 1.00 70.21 ATOM 480 C ALA 1520 1.699 22.159 9.922 1.00 70.21 ATOM 480 C ALA 1520 1.006 22.858 12.799 1.00 68.75 ATOM 490 C BLU 1522 1.0076 22.202 20.202 1.006 69.70 ATOM 490 C BLU 1522 1.0076	ATOM 440 0 ME1 151	0.612 33 22.087 1.00 46 20
ATOM 444 CB LEU 1516	ATOM 441 N 151	1 824 10 17.391 1.00 43 65
ATOM 444 CB LEU 1516  ATOM 445 CG LEU 1516  ATOM 446 CB LEU 1516  ATOM 447  ATOM 447  ATOM 448 CD LEU 1516  ATOM 448 CD LEU 1516  ATOM 448 CD LEU 1516  ATOM 449 OLEU 1516  ATOM 450 N LYS 1517  ATOM 450 N LYS 1517  ATOM 451 CG LYS 1517  ATOM 452 CA LYS 1517  ATOM 452 CD LYS 1517  ATOM 454 CG LYS 1517  ATOM 455 CD LYS 1517  ATOM 456 CE LYS 1517  ATOM 456 CE LYS 1517  ATOM 461 C LYS 1517  ATOM 462 O LYS 1517  ATOM 466 CE SER 1518  ATOM 466 C SER 1518  ATOM 467 CS SER 1518  ATOM 468 O SER 1518  ATOM 468 C SER 1518  ATOM 469 N ASP 1519  ATOM 471 CA ASP 1519  ATOM 472 CB ASP 1519  ATOM 474 O ASP 1519  ATOM 475 CA ALA 1520  ATOM 477 CA ALA 1520  ATOM 478 CB ALA 1520  ATOM 479 CB ALA 1520  ATOM 488 CB THR 1521  ATOM 488 CB THR 1521  ATOM 489 O THR 1521  ATOM 489 CB LYS 1523  ATOM 499 CB LYS 1523  ATOM 499 CB LYS 1523  ATOM 498 CA LYS 1523  ATOM 499 CB LY	ATOM 443 R LEU 1516	-0.053
ATOM 446 CB LEU 1516 ATOM 447 CD2 LEU 1516 ATOM 448 C LEU 1516 ATOM 449 CD LEU 1516 ATOM 449 CD LEU 1516 ATOM 449 CD LEU 1516 ATOM 450 N LYS 1517 ATOM 450 CB LEU 1516 ATOM 450 N LYS 1517 ATOM 450 CB LYS 1517 ATOM 460 CB SER 1518 ATOM 470 CB SER 1519 ATOM 471 CB ASP 1519 ATOM 472 CB ASP 1519 ATOM 473 CB SER 1519 ATOM 474 CB CB ASP 1519 ATOM 475 CB ASP 1519 ATOM 476 CB ASP 1519 ATOM 477 CB ALA 1520 ATOM 480 CB THR 1521 ATOM 490 CB LYS 1523 ATOM 490	ATOM 444 TEU 1516	40.8/2 1 00 .
ATOM 446 CD1 LEU 1516 ATOM 447 CD2 LEU 1516 ATOM 448 CD1 LEU 1516 ATOM 449 CD2 LEU 1516 ATOM 450 N LYS 1517 ATOM 450 N LYS 1517 ATOM 451 CA LYS 1517 ATOM 450 CD LYS 1517 ATOM 451 CD LYS 1517 ATOM 452 CA LYS 1517 ATOM 453 CB LYS 1517 ATOM 454 CD LYS 1517 ATOM 455 CD LYS 1517 ATOM 456 CE LYS 1517 ATOM 456 CE LYS 1517 ATOM 461 C LYS 1517 ATOM 462 C LYS 1517 ATOM 462 C LYS 1517 ATOM 463 N SER 1518 ATOM 465 CB SER 1518 ATOM 465 CB SER 1518 ATOM 465 CB SER 1518 ATOM 466 CB SER 1518 ATOM 467 C SER 1518 ATOM 468 C SER 1518 ATOM 468 C SER 1518 ATOM 469 N ASP 1519 ATOM 471 CA ASP 1519 ATOM 472 CB ASP 1519 ATOM 473 C ASP 1519 ATOM 474 C ASP 1519 ATOM 475 N ALA 1520 ATOM 476 CB ALA 1520 ATOM 478 CB ALA 1520 ATOM 478 CB ALA 1520 ATOM 479 C ALA 1520 ATOM 480 O THR 1521 ATOM 485 CG LYS 1527 ATOM 486 CG THR 1521 ATOM 487 CG THR 1521 ATOM 488 C THR 1521 ATOM 489 C ALA 1520 ATOM 494 C C SUJ 1522 ATOM 495 CB LYS 1523 ATOM 495 CB LYS 1523 ATOM 496 CB LYS 1523 ATOM 497 CB LYS 1523 ATOM 498 CA LYS 1523 ATOM 499 CB LYS 1523 AT	ATOM CB LEU 1516	16.175 16.448 1 20
ATOM 447 CD2 LEU 1516  ATOM 448 C LEU 1516  ATOM 449 O LEU 1516  ATOM 450 N LYS 1517  ATOM 450 N LYS 1517  ATOM 451 CE LYS 1517  ATOM 452 CA LYS 1517  ATOM 453 CB LYS 1517  ATOM 454 CG LYS 1517  ATOM 455 CD LYS 1517  ATOM 455 CD LYS 1517  ATOM 456 CE LYS 1517  ATOM 457 NZ LYS 1517  ATOM 461 C LYS 1517  ATOM 462 O LYS 1517  ATOM 463 N SER 1518  ATOM 466 CB SER 1518  ATOM 466 CB SER 1518  ATOM 466 CB SER 1518  ATOM 467 C SER 1518  ATOM 468 O SER 1518  ATOM 469 N ASP 1519  ATOM 471 CA ASP 1519  ATOM 472 CB ASP 1519  ATOM 473 C ASP 1519  ATOM 474 CB ASP 1519  ATOM 475 N ALA 1520  ATOM 478 CB ALA 1520  ATOM 478 CB ALA 1520  ATOM 488 C THR 1521  ATOM 488 C THR 1521  ATOM 489 C ALA 1520  ATOM 480 C ALYS 1523  ATOM 494 C GU ISS 1523  ATOM 495 C GU ISS 1523  ATOM 496 N LYS 1523  ATOM 497 C ALA 1520  ATOM 480 C ALYS 1523  ATOM 480 C ALYS 1523  ATOM 498 CA LYS 1523  ATOM 496 N LYS 1523  ATOM 496 N LYS 1521  ATOM 496 C GU ISS 1523  ATOM 496 C GU ISS 22 -2.478 21.800 6.761  ATOM 496 C GU ISS 22 -2.478 21.800 6.761  ATOM 496 C GU ISS 22 -2.478 21.800 6.761  ATOM 496 C GU ISS 22 -2.478 21.800 6.761  ATOM 496 C GU ISS 23 -2.478 21.800 6.761  ATOM 496 C GU ISS 23 -2.478 21.800 6.761  ATOM 496 C GU ISS 23 -2.478 21.800 6.761  ATOM 496 C GU ISS 23 -2.478 21.800 6.761  ATOM 496 C GU ISS 23 -2.478 21.800 6.761	ATOM 445 CG LEU 1516	16.917 15.374 1 00
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ATOM 449 O LEU 1516  ATOM 450 N LYS 1517  ATOM 452 CA LYS 1517  ATOM 453 CB LYS 1517  ATOM 454 CG LYS 1517  ATOM 455 CD LYS 1517  ATOM 455 CC LYS 1517  ATOM 455 CC LYS 1517  ATOM 456 CE LYS 1517  ATOM 457 NZ LYS 1517  ATOM 458 CE LYS 1517  ATOM 458 CE LYS 1517  ATOM 459 N SER 1518  ATOM 461 C LYS 1517  ATOM 462 N SER 1518  ATOM 463 N SER 1518  ATOM 465 CA SER 1518  ATOM 466 CB SER 1518  ATOM 467 C SER 1518  ATOM 468 O SER 1518  ATOM 467 C SER 1518  ATOM 468 O SER 1518  ATOM 470 CA ASP 1519  ATOM 471 CA ASP 1519  ATOM 472 CB ASP 1519  ATOM 473 CB ASP 1519  ATOM 474 O ASP 1519  ATOM 475 N ALA 1520  ATOM 478 CB ALA 1520  ATOM 479 C ALA 1520  ATOM 479 C ALA 1520  ATOM 480 O ALA 1520  ATOM 481 N THR 1521  ATOM 483 CA THR 1521  ATOM 483 CA THR 1521  ATOM 485 CG LYS 1523  ATOM 490 N GLU 1522  ATOM 490 N GLU 1522  ATOM 490 C GLU 1522  ATOM 496 C GLU 1522  ATOM 497 C GLU 1522  ATOM 498 CA LYS 1523  ATOM 496 CA LYS 1523  ATOM 496 CA LYS 1523  ATOM 496 CA LYS 1523  ATOM 497 CB LYS 1523  ATOM 498 CA LYS 1523  ATOM 499 CB LYS 1523  ATOM 500 CG LYS 1523  ATOM	Amou CD2 LEU 1516	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ATOM 450 N LEU 1516 ATOM 452 CA LYS 1517 ATOM 453 CB LYS 1517 ATOM 454 CG LYS 1517 ATOM 455 CD LYS 1517 ATOM 456 CC LYS 1517 ATOM 457 ATOM 458 CB LYS 1517 ATOM 458 CB LYS 1517 ATOM 459 CB LYS 1517 ATOM 450 CB LYS 1517 ATOM 451 CB LYS 1517 ATOM 452 CA LYS 1517 ATOM 455 CD LYS 1517 ATOM 456 CE LYS 1517 ATOM 457 ATOM 458 CB LYS 1517 ATOM 458 CB LYS 1517 ATOM 459 CB LYS 1517 ATOM 459 CB LYS 1517 ATOM 459 CB LYS 1518 ATOM 460 CB SER 1518 ATOM 461 CB SER 1518 ATOM 462 CB SER 1518 ATOM 463 CB SER 1518 ATOM 464 CB SER 1518 ATOM 465 CB SER 1518 ATOM 467 CB SER 1518 ATOM 468 CB SER 1518 ATOM 468 CB SER 1518 ATOM 471 CA ASP 1519 ATOM 472 CB ASP 1519 ATOM 473 CC ASP 1519 ATOM 473 CC ASP 1519 ATOM 474 O ASP 1519 ATOM 475 C ABP 1519 ATOM 475 C ABP 1519 ATOM 476 CB ALA 1520 ATOM 477 CA ALA 1520 ATOM 478 CB ALA 1520 ATOM 479 C ALA 1520 ATOM 488 C THR 1521 ATOM 488 C ATHR 1521 ATOM 489 C ALA 1520 ATOM 489 C ALA 1521 ATOM 489 C ALA 1521 ATOM 489 C ALA 1522 ATOM 490 C BLU 1522 ATOM 491 C GLU 1522 ATOM 492 CA GLU 1522 ATOM 493 CB GLU 1522 ATOM 494 C GLU 1522 ATOM 495 CB LYS 1523 ATOM 496 CB LYS 1523 ATOM 497 CB LYS 1523 ATOM 498 CB LYS 1523 ATOM 499 CB LYS 1523 ATOM 496 CB LYS 1523 ATOM 499 CB LYS 1523 ATOM 496	71 ON 448 C TEST	0.884 16 103 1.00 48.16
ATOM 452 CA LYS 1517 ATOM 453 CB LYS 1517 ATOM 454 CG LYS 1517 ATOM 455 CD LYS 1517 ATOM 455 CD LYS 1517 ATOM 456 CE LYS 1517 ATOM 457 ATOM 458 CG LYS 1517 ATOM 458 CG LYS 1517 ATOM 459 CB LYS 1517 ATOM 457 ATOM 457 ATOM 458 CG LYS 1517 ATOM 458 CG LYS 1517 ATOM 459 CB LYS 1517 ATOM 457 ATOM 458 CG LYS 1517 ATOM 458 CG LYS 1517 ATOM 459 CB LYS 1517 ATOM 459 CB LYS 1517 ATOM 461 C LYS 1517 ATOM 452 CB LYS 1517 ATOM 453 CB LYS 1517 ATOM 455 CD LYS 1517 ATOM 457 ATOM 458 CB LYS 1517 ATOM 458 CB LYS 1517 ATOM 459 CB ALA 1520 ATOM 479 CA ALA 1520 ATOM 479 CB ALA 1520 ATOM 488 CB THR 1521 ATOM 489 CB LYS 1522 ATOM 489 CG LYS 1523 ATOM 499 CB LYS 1523 ATOM 499 CB LYS 1523 ATOM 496 CB LYS 1523 ATOM 496 CG LYS 1523 ATOM 498 CB LYS 1523 ATOM 498 CB LYS 1523 ATOM 498 CB LYS 1523 ATOM 499 CB LYS 1523 ATOM 490 CG LYS 1523 ATOM 49	ATOM 449 0 TOTAL	0.810 17 110 1-00 42.80
ATOM 452 CA LYS 1517 ATOM 453 CB LYS 1517 ATOM 454 CG LYS 1517 ATOM 455 CD LYS 1517 ATOM 455 CD LYS 1517 ATOM 456 CE LYS 1517 ATOM 457 NZ LYS 1517 ATOM 461 C LYS 1517 ATOM 462 C LYS 1517 ATOM 463 N SER 1518 ATOM 465 CB SER 1518 ATOM 465 CB SER 1518 ATOM 466 CB SER 1518 ATOM 467 C SER 1518 ATOM 468 O SER 1518 ATOM 468 O SER 1518 ATOM 469 N ASP 1519 ATOM 471 CA ASP 1519 ATOM 472 CB ASP 1519 ATOM 473 C ASP 1519 ATOM 474 O ASP 1519 ATOM 475 N ALA 1520 ATOM 476 CB ALA 1520 ATOM 477 CA ALA 1520 ATOM 478 CB ALA 1520 ATOM 479 C ALA 1520 ATOM 488 C THR 1521 ATOM 489 O THR 1521 ATOM 489 C ALA 1520 ATOM 489 C ALA 1520 ATOM 489 C THR 1521 ATOM 499 C GLU 1522 ATOM 494 C GLYS 1523 ATOM 495 O GLU 1522 ATOM 495 O GLU 1522 ATOM 496 C GLYS 1523 ATOM 497 CB LYS 1523 ATOM 498 CA LYS 1523 ATOM 499 CB LYS 1523 ATOM 699 CB	450 N TWO	0.217 16 922 1 1.00 55.67
ATOM 453 CB LYS 1517 ATOM 454 CG LYS 1517 ATOM 455 CG LYS 1517 ATOM 455 CD LYS 1517 ATOM 456 CE LYS 1517 ATOM 457 NZ LYS 1517 ATOM 457 NZ LYS 1517 ATOM 467 NZ LYS 1517 ATOM 468 C LYS 1517 ATOM 468 C B SER 1518 ATOM 468 C SER 1518 ATOM 469 N ASP 1519 ATOM 471 CA ASP 1519 ATOM 473 C ASP 1519 ATOM 473 C ASP 1519 ATOM 474 O ASP 1519 ATOM 475 N ALA 1520 ATOM 477 CA ALA 1520 ATOM 477 CA ALA 1520 ATOM 478 CB ALA 1520 ATOM 479 C ALA 1520 ATOM 488 C THR 1521 ATOM 488 C THR 1521 ATOM 488 C THR 1521 ATOM 489 O ALA 1520 ATOM 489 O THR 1521 ATOM 489 C GLU 1522 ATOM 489 C GLU 1522 ATOM 489 C GLU 1522 ATOM 490 N GLU 1522 ATOM 490 C GLYS 1523 ATOM 690	ATOM 452 CA LVC	1.580 18 124 10.703 1.00 53.99
ATOM 455 CD LYS 1517 ATOM 456 CE LYS 1517 ATOM 457 NZ LYS 1517 ATOM 460 CE LYS 1517 ATOM 461 C LYS 1517 ATOM 462 O LYS 1517 ATOM 463 N SER 1518 ATOM 465 CB SER 1518 ATOM 466 CB SER 1518 ATOM 466 CB SER 1518 ATOM 467 C SER 1518 ATOM 468 O SER 1518 ATOM 468 O SER 1518 ATOM 468 O SER 1518 ATOM 470 CB ASP 1519 ATOM 471 CA ASP 1519 ATOM 472 CB ASP 1519 ATOM 473 C ASP 1519 ATOM 473 C ASP 1519 ATOM 474 O ASP 1519 ATOM 475 N ALA 1520 ATOM 477 CC ALA 1520 ATOM 478 CB ALA 1520 ATOM 488 C THR 1521 ATOM 489 CB THR 1521 ATOM 489 CB THR 1521 ATOM 489 CB GLU 1522 ATOM 494 C GGU 1522 ATOM 494 C GGU 1522 ATOM 495 N GGU 1522 ATOM 495 C GGU 1522 ATOM 496 C GLU 1522 ATOM 497 C GLU 1522 ATOM 498 CB LYS 1523 ATOM 499 CB LYS 1523 ATOM 500 CG LYS 1523 ATOM 500	ATOM 453 CD 131/	1 823 10 17.402 1.00 60 07
ATOM 455 CD LYS 1517 5.646 18.935 17.929 1.00 72.86 1.00 74.91 ATOM 456 CE LYS 1517 5.646 18.935 17.929 1.00 74.91 ATOM 461 C LYS 1517 8.010 18.241 17.649 1.00 75.45 1.00 74.91 ATOM 462 O LYS 1517 0.879 20.357 18.139 1.00 64.59 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.00 75.45 1.0	ATOM 454 CG 115	3 274 10 18.416 1.00 65 10
ATOM 456 CE LYS 1517	ATOM 455 CD 115	4 294 30 - 10.344 1.00 69 34
ATOM 457 NZ LYS 1517 6.688 17.851 18.197 1.00 74.91  ATOM 461 C LYS 1517 8.010 18.241 17.649 1.00 74.38  ATOM 462 O LYS 1517 0.879 20.357 18.139 1.00 65.97  ATOM 463 N SER 1518 0.303 20.451 17.649 1.00 65.97  ATOM 466 CB SER 1518 0.776 21.270 19.998 1.00 681.20  ATOM 466 CB SER 1518 0.002 23.322 20.202 18.00 681.20  ATOM 467 C SER 1518 0.144 23.222 20.202 18.00 681.20  ATOM 468 O SER 1518 0.144 23.222 20.202 18.00 681.20  ATOM 469 N ASP 1519 1.417 23.493 17.422 1.00 76.48  ATOM 471 CA ASP 1519 1.479 24.299 16.264 1.00 76.04  ATOM 473 C ASP 1519 1.799 24.299 16.264 1.00 76.48  ATOM 474 O ASP 1519 1.912 23.525 14.958 1.00 75.88  ATOM 475 C ALA 1520 1.486 22.265 14.958 1.00 77.52  ATOM 478 CB ALA 1520 1.486 22.265 14.958 1.00 77.52  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 73.06  ATOM 481 N THR 1521 1.440 22.015 11.401 1.00 69.15  ATOM 482 CB THR 1521 0.858 22.653 10.234 1.00 70.051  ATOM 483 CC THR 1521 0.858 22.653 10.234 1.00 70.051  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 73.48  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 73.48  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 73.48  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 70.051  ATOM 481 N THR 1521 1.440 22.015 11.401 1.00 69.15  ATOM 482 CB THR 1521 0.858 22.653 10.234 1.00 70.051  ATOM 489 CA GLU 1522 0.782 22.026 8.542 1.00 67.41  ATOM 490 N GLU 1522 0.782 22.026 8.607 1.00 70.051  ATOM 490 N GLU 1522 0.782 22.026 8.607 1.00 70.01  ATOM 491 C GLU 1522 0.782 22.026 8.607 1.00 67.41  ATOM 492 CA GLU 1522 0.782 22.026 8.607 1.00 67.41  ATOM 493 CB GLU 1522 0.782 22.026 8.607 1.00 67.41  ATOM 496 N LYS 1523 1.483 19.502 6.240 1.00 69.75  ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 68.75  ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63	ATOM 456 CD 213 1517	5.646 10 1 10.529 1.00 72 96
ATOM 461 C LYS 1517 8.010 18.241 17.649 1.00 74.38 ATOM 462 O LYS 1517 0.879 20.357 18.139 1.00 75.45 ATOM 463 N SER 1518 0.303 20.451 17.053 1.00 64.59 ATOM 465 CA SER 1518 0.776 21.270 19.098 1.00 68.20 ATOM 466 CB SER 1518 0.107 22.422 18.972 1.00 71.92 ATOM 468 O SER 1518 0.107 22.422 18.972 1.00 71.92 ATOM 469 N ASP 1519 0.142 23.247 17.718 1.00 74.68 ATOM 469 N ASP 1519 1.417 23.493 17.422 1.00 74.68 ATOM 471 CA ASP 1519 1.799 24.299 16.264 1.00 76.48 ATOM 472 CB ASP 1519 1.912 23.525 14.956 1.00 77.59 ATOM 473 C ASP 1519 1.912 23.525 14.956 1.00 77.52 ATOM 478 CB ALA 1520 1.486 22.265 14.956 1.00 73.06 ATOM 479 C ALA 1520 1.564 22.255 14.956 1.00 73.06 ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 73.06 ATOM 481 N THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 483 CA THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 484 CB THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 489 C THR 1521 3.053 23.815 10.043 1.00 72.38 ATOM 489 C THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 490 N GLU 1522 0.782 22.026 8.542 1.00 69.70 ATOM 491 C GLU 1522 0.782 22.026 8.542 1.00 69.70 ATOM 492 CA GLU 1522 0.782 22.026 8.542 1.00 69.70 ATOM 494 C GLU 1522 0.782 22.026 8.542 1.00 69.70 ATOM 495 N LYS 1523 0.512 20.419 6.827 1.00 69.75 ATOM 496 CB LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 496 CB LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 496 CB LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 496 CB LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 496 CB LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 497 CG LU 1522 0.718 20.024 7.168 1.00 60.75 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 60.75 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 60.75 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 60.75 ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63	ATOM 457 NO LYS 1517	6 686 18.935 17.929 1.00 74 91
ATOM 462 O LYS 1517	ATOM 1517	+0.197 7 30
ATOM 463 N SER 1518 0.303 20.451 17.053 1.00 64.59 ATOM 466 CB SER 1518 0.776 21.270 19.098 1.00 64.59 ATOM 466 CB SER 1518 0.776 21.270 19.098 1.00 64.59 ATOM 466 CB SER 1518 0.7002 23.322 20.202 1.00 69.89 ATOM 468 O SER 1518 0.144 23.247 17.718 1.60 71.92 ATOM 469 N ASP 1519 1.417 23.493 17.422 1.00 77.44 ATOM 471 CA ASP 1519 1.417 23.493 17.422 1.00 75.04 ATOM 473 C ASP 1519 1.799 24.299 16.264 1.00 77.59 ATOM 474 O ASP 1519 1.912 23.525 14.958 1.00 77.59 ATOM 475 N ALA 1520 1.486 22.265 14.958 1.00 77.59 ATOM 476 CB ALA 1520 1.486 22.265 14.958 1.00 77.52 ATOM 477 CA ALA 1520 1.486 22.265 14.958 1.00 77.30 ATOM 478 CB ALA 1520 0.930 20.079 14.010 1.00 73.06 ATOM 481 N THR 1521 1.440 22.015 11.401 1.00 73.06 ATOM 483 CA THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 484 CB THR 1521 1.950 23.110 9.272 1.00 70.05 ATOM 488 C THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 489 C THR 1521 1.950 23.110 9.272 1.00 70.05 ATOM 490 N GLU 1522 0.782 22.026 8.542 1.00 70.01 ATOM 490 N GLU 1522 1.663 9.932 1.00 70.21 ATOM 498 CA LYS 1523 1.683 1.00 69.70 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 67.41 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 60.63 ATOM 498 CA LYS 1523 1.483 19.502 6.247	ATOM ACC LYS 1517	18.241 17.649 1 (0)
ATOM 465 CA SER 1518	702 U LYS 1517	20.357 18.139 1 00 -
ATOM 466 CB SER 1518	70014 403 N SER 1519	20.451 17.053 1 22
ATOM 467 CB SER 1518 -0.002 23.322 20.202 1.00 68.20  ATOM 468 O SER 1518 -0.002 23.322 20.202 1.00 69.89  ATOM 468 O SER 1518 -0.798 23.604 17.006 1.00 74.68  ATOM 471 CA ASP 1519 1.417 23.493 17.422 1.00 76.48  ATOM 472 CB ASP 1519 1.417 23.493 17.422 1.00 76.48  ATOM 473 C ASP 1519 1.912 23.525 14.958 1.00 77.59  ATOM 474 O ASP 1519 1.912 23.525 14.958 1.00 77.59  ATOM 475 N ALA 1520 1.486 22.265 14.956 1.00 77.52  ATOM 478 CB ALA 1520 1.574 21.439 13.758 1.00 77.306  ATOM 479 C ALA 1520 0.930 20.079 14.010 1.00 73.06  ATOM 481 N THR 1521 0.889 22.153 12.598 1.00 73.06  ATOM 484 CB THR 1521 0.858 22.653 10.00 73.48  ATOM 485 OG1 THR 1521 0.858 22.653 10.234 1.00 70.21  ATOM 489 CG THR 1521 1.950 23.110 9.272 1.00 70.21  ATOM 489 CG THR 1521 0.015 21.616 9.550 1.00 70.23  ATOM 490 N GLU 1522 -0.782 22.026 8.542 1.00 69.70  ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 67.41  ATOM 496 N LYS 1523 1.483 19.502 6.240 1.00 69.70  ATOM 496 N LYS 1523 1.623 2.782 20.285 8.527 1.00 66.53  ATOM 496 N LYS 1523 1.623 2.782 20.286 8.542 1.00 67.41  ATOM 496 N LYS 1523 1.623 2.782 20.286 8.542 1.00 60.75  ATOM 496 CG LYS 1523 1.483 19.502 6.240 1.00 63.76  ATOM 496 CG LYS 1523 1.483 19.502 6.240 1.00 66.75  ATOM 496 CG LYS 1523 1.483 19.502 6.240 1.00 66.53  ATOM 496 CG LYS 1523 3.909 19.318 5.361 1.00 60.63	ATOM 465 CA SER 1518	21.270
ATOM 468 O SER 1518	400 CD CD	-0.107 22.422 19 232 1.00 68.2C
ATOM 469 N ASP 1518 -0.798 23.604 17.006 1.00 74.68 ATOM 471 CA ASP 1519 1.417 23.493 17.422 1.00 75.04 ATOM 473 C ASP 1519 1.799 24.299 16.264 1.00 76.48 ATOM 473 C ASP 1519 1.912 23.525 14.958 1.00 75.88 ATOM 475 N ALA 1520 2.374 24.075 13.959 1.00 77.59 ATOM 477 CA ALA 1520 1.486 22.265 14.956 1.00 77.59 ATOM 478 CB ALA 1520 0.930 20.079 14.010 1.00 73.06 ATOM 480 O ALA 1520 0.930 20.079 14.010 1.00 73.06 ATOM 481 N THR 1521 1.440 22.015 11.401 1.00 73.48 ATOM 483 CA THR 1521 1.440 22.015 11.401 1.00 69.15 ATOM 485 OGI THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 486 C THR 1521 2.505 21.969 8.607 1.00 72.71 ATOM 488 C THR 1521 3.053 23.815 10.00 77.01 ATOM 489 O THR 1521 -0.015 21.616 9.550 1.00 72.71 ATOM 489 C GLU 1522 -1.623 21.081 7.815 1.00 69.70 ATOM 494 C GLU 1522 -2.478 21.880 6.71 1.00 69.70 ATOM 495 O GLU 1522 -2.478 21.880 6.71 1.00 69.75 ATOM 496 N LYS 1523 1.483 19.502 6.240 1.00 60.75 ATOM 497 CB LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 69.75 ATOM 499 CB LYS 1523 3.909 19.318 5.361 1.00 60.63	467 C SED 15	-0.002 23 322 2 1.00 71.92
ATOM 471 CA ASP 1519 1.417 23.493 17.422 1.00 77.44  ATOM 472 CB ASP 1519 1.799 24.299 16.264 1.00 76.48  ATOM 473 C ASP 1519 3.126 25.011 16.539 1.00 77.59  ATOM 474 O ASP 1519 1.912 23.525 14.958 1.00 77.52  ATOM 475 N ALA 1520 1.486 22.265 14.956 1.00 74.39  ATOM 478 CB ALA 1520 1.574 21.439 13.758 1.00 72.93  ATOM 479 C ALA 1520 0.930 20.079 14.010 1.00 73.06  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 71.47  ATOM 481 N THR 1521 1.440 22.015 11.401 1.00 69.15  ATOM 483 CA THR 1521 1.950 23.110 9.272 1.00 70.21  ATOM 485 OG1 THR 1521 1.950 23.110 9.272 1.00 70.21  ATOM 487 CG2 THR 1521 2.505 21.969 8.607 1.00 72.71  ATOM 489 O THR 1521 3.053 23.815 10.043 1.00 72.71  ATOM 489 O THR 1521 3.053 23.815 10.043 1.00 72.71  ATOM 490 N GLU 1522 -0.782 22.026 8.542 1.00 70.21  ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 69.70  ATOM 494 C GLU 1522 -1.623 21.081 7.815 1.00 69.70  ATOM 495 O GLU 1522 -1.623 21.081 7.815 1.00 69.70  ATOM 496 N LYS 1523 0.512 20.249 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CB LYS 1523 3.909 19.318 5.361 1.00 62.47	468 O SED 350	0.144 23 247 - 1.00 69.89
ATOM 471 CA ASP 1519 1.417 23.493 17.422 1.00 76.44  ATOM 472 CB ASP 1519 1.799 24.299 16.264 1.00 76.48  ATOM 473 C ASP 1519 3.126 25.011 16.539 1.00 77.59  ATOM 474 O ASP 1519 1.912 23.525 14.958 1.00 75.88  ATOM 475 N ALA 1520 1.486 22.265 14.956 1.00 77.52  ATOM 477 CA ALA 1520 1.574 21.439 13.758 1.00 77.52  ATOM 478 CB ALA 1520 0.930 20.079 14.010 1.00 73.06  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 71.47  ATOM 481 N THR 1521 1.440 22.015 11.401 1.00 69.15  ATOM 484 CB THR 1521 0.858 22.653 10.234 1.00 70.05  ATOM 485 OG1 THR 1521 1.950 23.110 9.272 1.00 70.21  ATOM 488 C THR 1521 2.505 21.969 8.607 1.00 72.71  ATOM 489 O THR 1521 0.015 21.616 9.550 1.00 70.64  ATOM 490 N GLU 1522 -0.782 22.026 8.542 1.00 69.70  ATOM 493 CB GLU 1522 -0.782 22.026 8.542 1.00 69.70  ATOM 494 C GLU 1522 -0.782 22.026 8.542 1.00 69.70  ATOM 498 CA LYS 1523 0.512 1.8878 7.006 1.00 63.76  ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 60.63  ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 499 CB LYS 1523 3.909 19.318 5.361 1.00 60.63	469 N ACD 155	-0.798 23.604 37.005
ATOM 472 CB ASP 1519	471 CA 300	1.417 23 493 - 500 77.44
ATOM 473 C ASP 1.519	ATOM 472 CB ASD 1519	1.799 24 290 17.422 1.00 75.04
ATOM 474 O ASP 1519	ATOM 473 C 101	3 726 25 26 10.264 1.00 76 40
ATOM 475 N ALA 1520	ATOM 474 0 305	1 912 22 18.539 1.00 77 59
ATOM 477 CA ALA 1520 ATOM 478 CB ALA 1520 ATOM 479 C ALA 1520 ATOM 480 O ALA 1520 ATOM 481 N THR 1521 ATOM 483 CA THR 1521 ATOM 485 OGI THR 1521 ATOM 486 C THR 1521 ATOM 487 CG2 THR 1521 ATOM 488 C THR 1521 ATOM 489 O THR 1521 ATOM 489 C THR 1521 ATOM 490 N GLU 1522 ATOM 491 CG GLU 1522 ATOM 492 CA GLU 1522 ATOM 494 C GLU 1522 ATOM 495 O GLU 1522 ATOM 496 N LYS 1523 ATOM 496 N LYS 1523 ATOM 498 CA LYS 1523 ATOM 499 CB LYS 1523 ATOM 499 CG GLY 1523 ATOM 499 CG GLYS 1523 ATOM 499 CG LYS 1523 ATOM 500 CG LYS 1524 ATOM 500 CG ATOM 50.00 CG LYC 1.00 CO.00 CG LYC 1.00 CG LYC 1.00 CG LYC 1.00 CG LYC 1.00 CG LYC 1.0	ATOM 475 N ASP 1519	2 374 2 14.958 1.00 75 96
ATOM 478 CB ALA 1520 0.930 20.079 14.010 1.00 73.06  ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 71.47  ATOM 481 N THR 1521 0.096 22.858 12.797 1.00 73.48  ATOM 483 CA THR 1521 1.440 22.015 11.401 1.00 69.15  ATOM 484 CB THR 1521 0.858 22.653 10.234 1.00 70.05  ATOM 485 OGI THR 1521 1.950 23.110 9.272 1.00 70.21  ATOM 486 C THR 1521 2.505 21.969 8.607 1.00 72.71  ATOM 489 C THR 1521 3.053 23.815 10.043 1.00 71.01  ATOM 489 O THR 1521 0.015 21.616 9.550 1.00 70.64  ATOM 490 N GLU 1522 0.782 22.026 8.542 1.00 69.70  ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 67.41  ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 70.01  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50  ATOM 498 CA LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 500 CG LYS 1523 3.909 19.318 5.361 1.00 62.47	ATOM 477 CD 352	1.486 22 2. 13.959 1.00 77 52
ATOM 479 C ALA 1520 0.930 20.079 14.010 1.00 73.06 ATOM 480 O ALA 1520 0.889 22.153 12.598 1.00 71.47 ATOM 481 N THR 1521 1.440 22.015 11.401 1.00 69.15 ATOM 484 CB THR 1521 0.858 22.653 10.234 1.00 70.05 ATOM 485 OG1 THR 1521 1.950 23.110 9.272 1.00 70.21 ATOM 488 C THR 1521 2.505 21.969 8.607 1.00 70.21 ATOM 489 O THR 1521 3.053 23.815 10.043 1.00 71.01 ATOM 489 O THR 1521 0.015 21.616 9.550 1.00 70.64 ATOM 490 N GLU 1522 0.782 22.026 8.542 1.00 69.70 ATOM 493 CB GLU 1522 -0.782 22.026 8.542 1.00 69.70 ATOM 494 C GLU 1522 -1.623 21.081 7.815 1.00 67.41 ATOM 495 O GLU 1522 -2.478 21.800 6.761 1.00 70.01 ATOM 496 N LYS 1523 1.483 19.502 6.240 1.00 63.76 ATOM 498 CA LYS 1523 1.483 19.502 6.240 1.00 58.57 ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57 ATOM 499 CB LYS 1523 3.909 19.318 5.361 1.00 60.63	ATOM 479 CD ALM 1520	1 574 25 1.956 1.00 74 20
ATOM 480 O ALA 1520	ATOM 470 CB ALA 1520	0.930 20 23.758 1.00 72 83
ATOM 481 N THR 1521	ATOM 480 0 ALA 1520	0 889 22 14.010 1.00 73 06
ATOM 483 CA THR 1521 1.440 22.015 11.401 1.00 69.15  ATOM 484 CB THR 1521 0.858 22.653 10.234 1.00 70.05  ATOM 485 OG1 THR 1521 1.950 23.110 9.272 1.00 70.21  ATOM 488 C THR 1521 2.505 21.969 8.607 1.00 72.71  ATOM 489 O THR 1521 -0.015 21.616 9.550 1.00 70.64  ATOM 490 N GLU 1522 0.782 22.026 8.542 1.00 69.70  ATOM 493 CB GLU 1522 -0.782 22.026 8.542 1.00 69.70  ATOM 494 C GLU 1522 -1.623 21.081 7.815 1.00 67.41  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 67.41  ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 500 CG LYS 1523 3.909 19.318 5.361 1.00 60.63	ATOM ACT ALA 1520	22.153 12.598
ATOM 484 CB THR 1521	ATOM 481 N THR 1521	22.858 12.797
ATOM 485 OG1 THR 1521 1.950 23.110 9.272 1.00 70.05  ATOM 487 CG2 THR 1521 2.505 21.969 8.607 1.00 70.21  ATOM 488 C THR 1521 3.053 23.815 10.043 1.00 71.01  ATOM 489 O THR 1521 0.015 21.616 9.550 1.00 70.64  ATOM 490 N GLU 1522 -0.782 22.026 8.542 1.00 69.70  ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 67.41  ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 70.01  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50  ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63	ATOM 483 CA THR 1521	22.015 11.401 1 00 73.48
ATOM 487 CG2 THR 1521 2.505 21.969 8.607 1.00 70.21  ATOM 488 C THR 1521 3.053 23.815 10.043 1.00 71.01  ATOM 489 O THR 1521 -0.015 21.616 9.550 1.00 70.64  ATOM 490 N GLU 1522 -0.782 22.026 8.542 1.00 69.70  ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 67.41  ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 70.01  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50  ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63	304 CB THR 1521	22.653 10.234 1 00
ATOM 488 C THR 1521 3.053 23.815 10.043 1.00 72.71 ATOM 489 O THR 1521 -0.015 21.616 9.550 1.00 70.64 ATOM 490 N GLU 1522 -0.782 22.026 8.542 1.00 69.70 ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 67.41 ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 70.01 ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50 ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 69.75 ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 63.76 ATOM 499 CB LYS 1523 2.782 20.230 5.883 1.00 60.63 ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63	ATOM 485 OG1 THR 1521	23.110 9.272 1 00
ATOM 488 C THR 1521	AMON: 487 CG2 THR 1527	2.505 21.969 8 607
ATOM 490 N GLU 1522 -0.782 22.026 8.542 1.00 69.70 ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 67.41 ATOM 494 C GLU 1522 -0.718 20.024 7.168 1.00 67.41 ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50 ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 69.76 ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57 ATOM 499 CG LYS 1523 2.782 20.230 5.883 1.00 60.63 ATOM 500 CG LYS 1523 3.909 19.318 5.361 1.00 62.47		3.053 23 836 1.00 72.71
ATOM 492 CA GLU 1522 -0.782 22.026 8.542 1.00 70.64  ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 69.70  ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 70.01  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50  ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CG LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 500 CG LYS 1523 3.909 19.318 5.361 1.00 62.47	489 O TUD	-0.015 21 616
ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 69.70  ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 70.01  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50  ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CG LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 500 CG LYS 1523 3.909 19.318 5.361 1.00 62.47	490 N GLU 1533	0.015 20 443
ATOM 493 CB GLU 1522 -1.623 21.081 7.815 1.00 69.70  ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 70.01  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50  ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 499 CG LYS 1523 2.782 20.230 5.883 1.00 60.63  ATOM 500 CG LYS 1523 3.909 19.318 5.361 1.00 62.47	ATOM 492 Ch Cr.	-0.782 22 026 1.00 72.38
ATOM 494 C GLU 1522 -2.478 21.800 6.761 1.00 67.41  ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 64.50  ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75  ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57  ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63  3.909 19.318 5.361 1.00 62.47	ATOM 493 CB CT:	-1.623 21 081 8.542 1.00 69.70
ATOM 495 O GLU 1522 -0.718 20.024 7.168 1.00 70.01 ATOM 496 N LYS 1523 0.512 20.419 6.827 1.00 60.75 ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57 ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63 3.909 19.318 5.361 1.00 62.47	ATOM 494 C CTV	-2.478 21 ROO815 1.00 67.41
ATOM 496 N LYS 1523	ATOM 495 0	-0 719 22 0./61 1.00 70 02
ATOM 498 CA LYS 1523 0.512 20.419 6.827 1.00 63.76 ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 58.57 ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63 3.909 19.318 5.361 1.00 62.47	ATOM 406 TO GLU 1522	-1 125 10 a= 7.168 1.00 64 50
ATOM 499 CB LYS 1523 1.483 19.502 6.240 1.00 60.75 ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63 3.909 19.318 5.361 1.00 62 47	ATOM 490 T LYS 1523	0.512 20 7.006 1.00 63 76
ATOM 500 CG LYS 1523 2.782 20.230 5.883 1.00 60.63 3.909 19.318 5.361 1.00 62 47	ATOM 490 CA LYS 1523	0.512 20.419 6.827 1 00
3.909 19.318 5.361 1.00 60.63 5.361 1.00 62 47	ATOM CB LYS 1523	19.502 6.240 1 00 -
19.318 5.361 1.00 62 47		5.883 7 00 5
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	SSSD/55145, v01	1.00 62.47

MOTA	501	CD	LYS	1523	3.459	18.461	4.168		63.35
ATOM	502	CE	LYS	1523	4.633	17.700	3.559	1.00	66.57
MOTA	503	NZ	LYS	1523	4.210	16.733	2.498	1.00	69.56
MOTA	507	C	LYS	1523	1.763	18.441	7.281	1.00	55.98
MOTA	508	0	LYS	1523	1.790	17.251	6.972	1.00	56.37
ATOM	509	N	ASP	1524	1.960	18.885	8.517	1.00	52.16
ATOM	511	CA	ASP	1524	2.211	17.980	9.630		48.91
ATOM	512	CB	ASP	1524	2.487	18.762	10.915	1.00	50.87
MOTA	513	CG	ASP	1524	3.865	19.401	10.928	1.00	53.00
ATOM	514	OD1	ASP	1524	4.004	20.511	11.489	1.00	53.77
MOTA	515	OD2	ASP	1524	4.816	18.785	10.394	1.00	56.30
MOTA	516	С	ASP	1524	1.032	17.031	9.831	1.00	45.34
ATOM	517	0	ASP	1524	1.221	15.858	10.176		45.63
ATOM	518	N	LEU	1525	-0.176	17.530	9.593		40.15
ATOM	520	CA	LEU	1525	-1.368	16.715	9.711		39.38
ATOM	521	CB	LEU	1525	-2.624	17.588	9.633		41.66
MOTA	522	C'G	LEU	1525	-4.020	16.937	9.585		42.75
ATOM	<b>5</b> 23	CD1	LEU	1525	-4.245	15.945	10.727	1.00	
ATOM	524	CD2	LEU	1525	-5.058	18 026	9.644	1.00	
ATOM	525	С	LEU	1525	-1.340	15.699	8.575	1.00	39.77
MOTA	526	O	LEU	1525	-1.509	14.506	8.813	1.00	39.11
ATOM	527	N	SER	1526	-1.062	16.172	7.361		39.64
ATOM	529	CA	SER	1526	-0.998	15.320	6.181		40.65
ATOM	530	CB	SER	1526	-0.541	16.105	4.947		43.32
ATOM	531	OG	SER	1526	-1.398	17.190	4.656		52.41
ATOM	533	C,	SER	1526	-0.015	14.201	6.383	1.00	39.12
ATOM	534	O	SER	1526	-0.346	13.038	6.198	1.00	41.75
ATOM	535	N	ASP	1527	1.203	14.553	ö.769	1.00	38.30
MOTA	537	CA	ASP	1527	2 244	13.552	6.969	1.00	39.28
MOTA	538	CB	ASP	1527	3.531	14.208	7.47:	1.00	41.16
ATOM	539	C'G	ASP	1527	4.218	15.069	6.404	1.00	45.20
ATOM	540	OD1	ASP	1527	3.861	14.972	5.198		43.25
ATOM	541	OD2	ASP	1527	5.132	15.840	6.788		45.93
ATOM	542	C	ASP	1527	1.788	12.443	7.903	1.00	37.34
ATOM	543	0	ASP	1527	1.867	11.259	7.557	1.00	37.24
ATOM	544	N	LEU	1528	1.224	12.535	9.036	1.00	35.88
MOTA	546	CA	LEU	1528	0.728	11.874	10.009	1.00	35.07
ATOM	547	CB	LEU	1528	0.185	12.606	11.242	1.00	34.38
ATOM	548	CG	LEU	1528	-0.146	11.789	12.491	1.00	35.86
MOTA	549	CD1	LEU	1528	1.009	10.845	12.820	1.00	34.83
MOTA	550	CD2	LEU	1528	-0.435	12.711	13.642	1.00	29.98
ATOM	551	C	LEU	1528	-0.351	10.977	9.374	1.00	33.31
MOTA	552	0	LEU	1528	-0.342	9.756	9.552	1.00	34.55
ATOM	553	N	ILE	1529	-1.236	11.575	8.585	1.00	32.16
ATOM	555	CA	ILE	1529	-2.306	10.829	7.924	1.00	30.94
MOTA	556	CB	ILE	1529	-3.304	11.757	7.178	1.00	
ATOM	557	CG2	ILE	1529	-4.388	10.926	5.521	1.00	
A'TOM	558	CG1	ILE	1529	-3.953	12.723	8.169	1.00	
MOTA	559	CD1	ILE	1529	-4.877	13.736	7.526	1.00	
ATOM	560	С	ILE	1529	-1.684	9.856	6.947	1.00	
ATOM	561	0	ILE	1529	-2.058	8.683	6.912	1.00	
MOTA	562	N	SER	1530	-0.703	10.331	6.191	1.00	

ATOM	_	64	CA S	SER	1530	0.00	0.7	0 40			
ATOM	_	65	CB S	SER	1530	1.10		9.49 10.30			32.04
ATOM	5	66	OG S	SER	1530	0.59		11.50			35.20
ATOM	5	68	C S	ER	1530	0.62					41.97
ATOM	56	69	0 5	ER	1530	0.47		8.26			29.06
ATOM	5.	70	N G	LU	1531	1.28		7.14			26.64
ATOM	5 7	72	CA G	LU	1531	1.20		8.46			23.86
ATOM	57	73 (	CB G	LU	1531			7.36			23.86
ATOM	57	74 (	CG G	LU	1531	2.72		7.89			25.69
ATOM	57			LU	1531	3.50		6.80			23.65
ATOM	57	6 (	El G		1531	4.34		7.319			26.03
ATOM	57		)E2 G		1531	4.92		6.473			25.92
ATOM	57			บับ	1531	4.43		8.549		4 1.00	26.55
ATOM	57	9 0		מב	1531	0.90		6.325			25.44
ATOM	58	0 N			1532	1.200		5.126			23.67
ATOM	58:		A MI		1532	-0.289		6.788			26.39
ATOM	58:		B ME		1532	-1.365		5.898	_		26.57
ATOM	584	_			1532	-2.473		6.720	9.71		24.81
ATOM	589	_			1532	-3.645		5.889	10.19	1 1.00	27.47
ATOM	586					-4.969		5.899	10.86		28.43
ATOM	587		ME		1532	-5.178		8.102	9.576	1.00	
ATOM	588		ME		1532	-1.923		5.076	7.863		
ATOM	589	_	GL		1532	-2.048		3.850	7.933	1.00	
ATOM	591				1533	-2.221		5.760	6.762	1.00	
ATOM	592				1533	-2.732		5.111	5.565	1.00	
ATOM	593				1533	-2.983		6.143	4.476		
ATOM	594				1533	-4.064		7.127	4.852	1.00 2	
ATOM	595				1533	-5.402		6.461	5.119	_	
ATOM	596		1 GLI 2 GLI		1533	-5.913		5.745	4.240	1.00 2	
ATOM	597	C	GLt		1533	-5.964		6.6€2	6.209	1.00 3	0 00
ATOM	598	0	GLU		1533	-1.723		4.089	5.093	1.00 3	
ATOM	599	N	MET		1533	-2.080		2.983	4.706	1.00 3	
ATOM	601	CA			1534	-0.455		4.472	5.166	1.00 3	
ATOM	602	CB	MET		1534	0.664		3.618	4.793	1.00 3	
ATOM	603	CG	MET	_	1534	1.957		4.390	5.003	1.00 3	
ATOM	604	SD	MET	_	1534	3.159		3.559	4.851	1.00 3	
ATOM	605	CE	MET		1534	3.577		3.513	3.164	1.00 5	
ATOM	606	CE	MET		1534	5.153		4.319	3.204	1.00 4	
ATOM	607	0	MET MET	-	.534	0.670	:	2.373	5.681	1.00 3	
ATOM	608	N	MET		.534	0.816	:	1.250	5.198	1.00 33	
ATOM	610	CA			535	0.509	2	2.571	6.982	1.00 30	3.76
ATOM	611	CB	MET		535	0.469	1	l.453	7.902	1.00 28	
ATOM	612		MET		535	0.419	1	1.946	9.352	1.00 24	75
ATOM	613	CG	MET		535	1.717	2	2.540	9.850	1.00 21	E. 7.5
ATOM		SD	MET		535	1.722	2	2.764	11.628	1.00 22	
ATOM	614	CE	MET		535	1.681			11.727	1.00 22	.97
ATOM	615	С	MET		535	-0.725		.540	7.572	1.00 30	
ATOM	616	0	MET		535	-0.636		.694	7.706	1.00 30	. 3 3
ATOM	617	N	LYS		536	-1.823		.135	7.104	1.00 28	
ATOM	619	CA	LYS		536	-3.011		.364	6.732	1.00 28	. 71
ATOM ATOM	620	CB	LYS		536	-4.176		. 289	6.413	1.00 28	. 0 /
ATOM	621	CG	LYS		536	-4.689		.080	7.579	1.00 25	. 54
AT ON	622	CD	LYS	15	36	-5.810		.979	7.127	1.00 21	
								-	/	±.00 19	. 69

ATOM	623	CE	LYS	1536	-6.414	3.717	8.288	1.00	23.50
ATOM	624	NZ	LYS	1536	-7.469	4.668	7.850	1.00	23.53
MOTA	628	C	LYS	1536	-2.765	-0.542	5.530	1.00	29.09
MOTA	629	0	LYS	1536	-3.127	-1.708	5.550	1.00	34.02
ATOM	630	N	MET	1537	-2.141	-0.009	4.488	1.00	29.03
ATOM	632	CA	MET	1537	-1.869	-0.792	3.288	1.00	30.13
ATOM	633	CB	MET	1537	-1.315	0.111	2.177		31.96
ATOM	634	CG	MET	1537	-2.304	1.114	1.589		35.15
MOTA	635	SD	MET	1537	-3.757		0.787		41.18
ATOM	636	CE	MET	1537	-3.026	-0.360	-0.666		43.05
ATOM	637	С	MET	1537	-0.905	-1.946	3.531	1.00	30.22
ATOM	638	0	MET	1537	-1.118	-3.051	3.045		30.88
ATOM	639	N	ILE	1538	0.164	-1.686	4.275		30.91
MOTA	641	CA	ILE	1538	1.192		4.536		30.29
ATOM	642	CB	ILE	1538	2.429		5.221		28.64
ATOM	643	CG2	ILE	1538	3.493		5.453		29.84
ATOM	644	CG1	ILE	1538	3.025		4.287		32.82
MOTA	645	CD1	ILE	1538	4.358		4.763		38.38
ATOM	646	C	ILE	1538	0.759		5.237		29.07
ATOM	647	0	ILE	1538	1.229		4.876		28.30
ATOM	648	N	GLY	1539	-0.178		6.174		27.61
ATOM	650	CA	GLY	1539	-0.592	-5.147	6.849		26.22
ATOM	651	С	GLY	1539	0.273	-5.484	8.055		25.67
ATOM	652	Ō	GLY	1.539	1.345		8.241		28.05
ATOM	653	N	LYS	1540	-0.150		8.819		23.80
ATOM	655	CA.	LYS	1540	0.532	-6.876	10.046		21.77
ATOM	656	СВ	LYS	1540	-0.491	-7.436	11.045		20.04
ATOM	657	CG	LYS	1540	-1.505	-6.435	11.480		24.45
ATOM	658	CD	LYS	1540		-6.997	12.488		32.57
ATOM	659	CE	LYS	1540	-3.516	-5.946	12.882		35.05
ATOM	660	NZ	LYS	1540	-2.959	-4.850	13.733	1.00	39.81
ATOM	664	C	LYS	1540	1.669	-7.862	9.958	1.00	
ATOM	665	0	LYS	1540	1.671	-8.738	9.099		21.80
ATOM	666	N	HIS	1541	2.626	-7.722	10.876		19.98
ATOM	668	CA	HIS	1541	3.770	-8.626	11.000		22.43
ATOM	669	CB	HIS	1541	4.854	-8.374	9.965		22.34
ATOM	670	CG	HIS	1541	5.892	-9.455	9.923		20.68
ATOM	671		HIS	1541	5.906	-10.654	9.295		20.60
ATOM	672		HIS	1541	7.074		10.633		
ATOM	674		HIS	1541		-10.490	10.444		23.35
ATOM	675		HIS	1541		-11.278	9.634		22.04
ATOM	677	C	HIS	1541	4.385	-8.477	12.376		
ATOM	678	ō	HIS	1541	4.538	-7.367	12.885		27.21
ATOM	679	N	LYS	1542	4.726	-9.619	12.958		31.33
ATOM	681	CA	LYS	1542	5.319	-9.698	14.285		
ATOM	682	CB	LYS	1542					30.39
ATOM	683	CG	LYS			-11.151	14.610		33.76
ATOM	684	CD	LYS	1542		-11.370 -12.833	15.994		42.16
ATOM	685	CE		1542			16.230		49.69
ATOM	686	NZ	LYS	1542		-13.499	14.988		57.71
ATOM	690		LYS	1542		-14.904	15.237		62.05
		С	LYS	1542	6.515	-8.808	14.462		27.21
ATOM	691	0	LYS	1542	6.690	-8.232	15.522	1.00	29.68





MOTA	755	N	ALA	1550	-7.369	4.143	15.530	1.00 27.34
MOTA	757	CA	ALA	1550	-7.212	5.582	15.414	1.00 25.85
MOTA	758	CB	ALA	1550	-6.925	5.947	13.978	1.00 23.09
ATOM	759	C	ALA	1550	-8.430	6.353	15.897	1.00 26.58
MOTA	760	0	ALA	1550	-9.562	5.866	15.797	1.00 28.26
MOTA	761	N	CYS	1551	-8.182	7.551	16.429	1.00 26.30
ATOM	763	CA	CYS	1551	-9.227	8.471	16.899	1.00 28.29
MOTA	764	CB	CYS	1551	-8.966	8.952	18.342	1.00 27.12
ATOM	765	SG	CYS	1551	-9.101	7.681	19.630	1.00 27.09
MOTA	766	C	CYS	1551	-9.092	9.646	15.934	1.00 28.57
ATOM	767	0	CYS	1551	-8.156	10.436	16.044	1.00 26.80
MOTA	768	N	THR	1552	-9.966	9.699	14.933	1.00 29.27
MOTA	770	CA	THR	1552	-9.889	10.736	13.921	1.00 29.30
MOTA	771	CB	THR	1552	- 9 . 779	10.110	12.495	1.00 27,19
ATOM	772	OG1	THR	1552	-10.978	9.393	12.191	1.00 26.68
ATOM	774	CG2	THR	1552	-8.629	9.133	12.414	1.00 27.00
MOTA	775	C	THR	1552	-11.045	11.716	13.905	1.00 29.86
MOTA	776	0	THR	1552	-10.918	12.838	13.403	1.00 30.69
ATOM	777	N	GLN	1553	-12.201	11.268	14.369	1.00 31 21
ATOM	779	CA	GLN	1553	-13.374	12.124	14.329	1.00 34.31
ATOM	780	CB	GLN	1553	-14.641	11.279	14.147	1.00 33.00
MOTA	781	CG	GLN	1553	-14.714	10.530	12.820	1.00 34.68
MOTA	782	CD	GLN	1553	-14.584	11.453	31.617	1.00 39.26
ATOM	783	OE1	GLN	1553	~15.300	12.449	11.506	1.00 43.55
MOTA	784	NE2	GLN	1553	-13.668	11.129	1.0.718	1.00 37.56
ATOM	787	C	GLN	1553	-13.502	13.040	15.526	1.00 36.86
MOTA	788	0	GLN	1553	-13.030	1.2.714	16.613	1.00 34.88
ATOM	789	N	ASP	1554	-14.122	14.195	15.290	1.00 40.73
MOTA	791	CA	ASP	1554	-14.369	15.202	16.3:3	1.00 42.49
ATOM	792	CB	ASP	1554	-15.693	14.913	17.028	1.00 46.26
MOTA	793	CG	ASP	1554	-16.907	15.174	16.153	1.00 51.14
MOTA	794	OD1	ASP	1554	-17.686	16.097	16.488	1.00 57.62
ATOM	795	OD2	ASP	1554	-17.092	14.463	15.146	1.00 55.72
ATOM	796	C	ASP	1554	-13.249	15.299	17.336	1.00 42.31
MOTA	797	0	ASP	1554	-13.443	14.955	18.501	1.00 43.61
MOTA	798	N	GLY	1555	-12.077	15.753	16.902	1.00 41.03
ATOM	800	CA	GLY	1555	-10.960	15.864	17.823	1.00 37.98
MOTA	801	C	GLY	1555	-9.605	15.674	17.167	1.00 38.30
ATOM	802	0	GLY	1555	-9.533	15.478	15.953	1.00 37.28
ATOM	803	N	PRO	1556	-8.511	15.693	17.961	1.00 37.62
ATOM	804	CD	PRO	1556	-8.575	15.755	19.429	1.00 37.23
ATOM	805	CA	PRO	1556	-7.123	15.533	17.500	1.00 33.79
ATOM	806	CB	PRO	1556	-6.296	15.748	18.773	1.00 33.33
MOTA	807	CG	PRO	1556	-7.254	16.353	19.770	1.00 36.99
MOTA	808	C	PRO	1556	-6.891	14.134	16.990	1.00 33.57
MOTA	809	0	PRO	1556	-7.378	13.175	17.568	1.00 32.10
ATOM	810	N	LEU	1557	-6.168	14.031	15.884	1.00 33.23
MOTA	812	CA	LEU	1557	-5.859	12.745	15.300	1.00 34.20
MOTA	813	CB	LEU	1557	-5.173	12.950	13.944	1.00 32.88
MOTA	814	CG	LEU	1557	-4.674	11.716	13.183	1.00 29.78
ATOM	815	CD1	LEU	1557	-5.810	10.730	12.943	1.00 29.22
ATOM	816	CD2	LEU	1557	-4.085	12.161	11.880	1.00 28.17

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AT(	- J.	EU 1557	-4.950 11.927 16.225
ATO	0 101	ម 1557	10.225 1.00 36.29
ATO	0.7.2 14 1.7		5 427 12.365 16.580 1.00 37 50
ATC	OFT CA TY		10.705 16.658 1.00 35 35
ATO	V22 CB 110		3.890 17.495 1.00 33 00
ATO	M 823 CG TV		3.516 18.805 1 00 34 16
ATO	M 824 CD1 TV	•	-5.363 10.629 19.806 1 00 34 40
ATO	<sup>M</sup> 825 CE1 ການ		-6.364 10.688 20.771 1.00 32 22
ATO	M 826 CD2 Trv	_	-6.438 11.747 21.663 1 00 21.7
ATO	M 827 CE2 TY		-4.426 11.655 19 757 1 00 an
ATOM	4 828 CZ TY		-4.488 12.715 20 640 1 00 37.30
ATOM	829 OH TY	-555	-5.494 12.762 21 597 1 00
ATOM			-5.561 13.848 22 431 1 22
ATOM			-4.379 9 607
ATOM	022		-5.379 7.000
ATOM	0.2 =		-3.109 B 33
ATOM	035 CA VAL	-005	-2.727 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ATOM	JAV GD VAL	1559	-1.647 7.426
ATOM	-4- 170	1559	-1.281 6.140
ATOM	838 CG2 VAL	1559	-2 147 0 FOR 13.326 1.00 24 36
ATOM	839 C VAL	1559	-2 239 ( 200 17.765 1.00 19.21
ATOM	840 O VAL	1559	-1.169 6 25.65
ATOM	841 N ILE	1560	-3.067 5.005 1.00 24.97
ATOM	843 CA ILE	1560	-2.777 4.060 17.046 1.00 25.91
ATOM	844 CB ILE	1560	-4.081 3.535 18.042 1.00 26.94
ATOM	845 CG2 ILE	1560	3.530 18.637 1.00 24.89
	846 CG1 ILE	1560	-5 020 2.744 L9.900 1.00 17.89
ATOM	847 CD1 ILE	1560	18.967 1.00 22.84
ATOM	848 C ILE	1560	1 055 4.304 19.163 1.00 22.51
ATOM	849 O ILE	1560	2 445 2.896 17.467 1.00 30.61
ATOM	850 N VAL	1561	0.600 2.411 16.636 1.00 31.41
ATOM	852 CA VAL	1561	0 222 2.811 17.890 1.00 30.26
ATOM	853 CB VAL	1561	1 466 1.779 17.429 1.00 29.39
ATOM	854 CG1 VAL	1.561	1 070 2.437 16.730 1.00 30.18
ATOM	855 CG2 VAL	1561	3.188 15.475 1.00 20 60
ATOM	000	1561	3.415 17.675 1.00 32 92
ATOM	000 -	1561	18.588 1.00 27 40
ATOM	0.00	1562	0.323 1.128 19.742 1 00 39 72
ATOM	0.00	1562	1.381 -0.209 18.279 1 00 24 75
ATOM	861 05	1562	19.308 1.00 22 64
ATOM	060 55	1562	2.426 -2.410 18.676 1 00 17 00
ATOM	863 CD	562	1.365 -3.282 18.029 1 00 24 22
ATOM	P64 07-	.562	1.909 -4.552 17 393 1 00 01
ATOM	0.65		1.247 ~5.592 17 507 1 00 77
ATOM	966 0	562	2.974 -4.538 16 722 1 00 05
ATOM	967 0	562	2.885 -0.534 20.259 1 00 25.62
ATOM	860 17 -	562	3.638 0.355 19.899 1.00 25.09
ATOM	970 03	563	2 897 1 202 1.00 23.82
ATOM	971 65 -	563	3 805 0 500
ATOM	872 55	563	3 045 0 400 26.93
ATOM	977 001	563	3 868 0 000 27.19
ATOM	974 675	563	4 581 1 106 27.72
ATOM		563	5 303 1 505 24.976 1.00 30.61
	875 CD2 TYR 15	63	3 908 0 755
			3.908 -0.753 26.176 1.00 25.77

ATOM	876	CE2	TYR	1563	4.626	-0.344	27.267	1.00 26.81
ATOM	877	CZ	TYR	1563	5.329	0.845	27.210	1.00 32.81
ATOM	878	OH	TYR	1563	6.091	1.271	28.276	1.00 40.16
MOTA	880	С	TYR	1563	4.989	-1.487	22.675	1.00 28.73
MOTA	881	0	TYR	1563	4.815	-2.704	22.735	1.00 27.05
MOTA	882	N	ALA	1564	6.189	-0.908	22.743	1.00 29.89
ATOM	884	CA	ALA	1564	7.453	-1.634	22.916	1.00 28.50
ATOM	885	CB	ALA	1564	8.392	-1.349	21.721	1.00 27.54
ATOM	886	С	ALA	1564	8.036	-1.092	24.229	1.00 27.05
ATOM	887	0	ALA	1564	8.790	-0.129	24.249	1.00 31.20
ATOM	888	N	SER	1565	7.650	-1.706	25.333	1.00 27.11
MOTA	890	CA	SER	1565	8.062	-1.251	26.652	1.00 28.91
MOTA	891	CB	SER	1565	7.501	-2.152	27.729	1.00 27.33
MOTA	892	OG	SER	1565	8.108	-3.419	27.650	1.00 26.58
ATOM	894	С	SER	1565	9.530	-1.085	26.915	1.00 30.19
ATOM	895	0	SER	1565	9.897	-0.330	27.810	1.00 33.44
MOTA	896	N	LYS	1566	10.368	-1.801	26.178	1.00 30.99
ATOM	898	CA	LYS	1566	11.798	-1.708	26.410	1.00 30.50
ATOM	899	CB	LYS	1566	12.452	-3.082	26.335	1.00 30.38
ATOM	900	CG	LYS	1566	12.037.	-3.943	27.507	1.00 27.83
ATOM	901	CD	LYS	1566	12.605	-5.33 <i>9</i>	27.457	1.00 32.36
ATOM	902	CE	LYS	1566	12.345	-6.024	28.784	1.00 30.57
ATOM	903	NZ	LYS	1566	12.651	-7.460	28.722	1.00 34.82
ATOM	907	C	LYS	1566	12.526	-0.678	25.573	1.00 30.39
ATOM	908	0	LYS	1566	13.755	-0.567	25.640	1.00 32.53
ATOM	909	N	GLY	1567	11.753	0.1.27	24.851	1.00 29.45
MOTA	911	CA	GLY	1567	12.319	1.184	24.035	1.00 29.17
ATOM	912	C	GL.Y	1567	13.079	0.742	22.806	1.00 28.14
MOTA	913	೦	GLY	1567	12.875	-0.364	22.324	1.00 27.70
MOTA	914	N	ASN	1568	13.975	1.601	22.320	1.00 29.48
ATOM.	916	CA	ASN	1568	14.754	1.308	21.121	1.00 30.00
ATOM	917	CB	ASN	1568	15.271	2.591	20.464	1.00 28.53
ATOM	918	ÇG	ASN	1568	16.342	3.285	21.281	1.00 30.13
MOTA	919	OD1	ASN	1568	17.305	2.670	21.730	1.00 31.50
ATOM	920	ND2	ASN	1568	16.212	4.591	21.420	1.00 30.91
MOTA	923	C	ASN	1568	15.892	0.333	21.352	1.00 28.83
MOTA	924	0	ASN	1568	16.371	0.201	22.472	1.00 29.87
MOTA	925	N	LEU	1569	16.346	-0.300	20.274	1.00 27.43
MOTA	927	CA	LEU	1569	17.417	-1.291	20.323	1.00 29.95
ATOM	928	CB	LEU	1569	17.511	-2.022	18.972	1.00 28.96
MOTA	929	CG	LEU	1569	18.508	-3.173	18.797	1.00 30.82
MOTA	930		LEU	1569	18.431	-4.211	19.939	1.00 28.31
ATOM	931	CD2	LEU	1569	18.244	-3.819	17.461	1.00 25.70
ATOM	932	С	LEU	1569	18.805	-0.779	20.754	1.00 29.74
ATOM	933	0	LEU	1569	19.530	-1.484	21.447	1.00 28.35
MOTA	934	N	ARG	1570	19.179	0.427	20.341	1.00 31.42
ATOM	936	CA	ARG	1570	20.485	0.985	20.703	1.00 32.81
MOTA	937	CB	ARG	1570	20.639	2.395	20.115	1.00 31.01
MOTA	938	CG	ARG	1570	21.922	3.091	20.543	1.00 35.33
MOTA	939	CD	ARG	1570	21.918	4.581	20.212	1.00 38.30
MOTA	940	NE	ARG	1570	20.700	5.272	20.649	1.00 47.77
ATOM	942	CZ	ARG	1570	20.393	5.595	21.912	1.00 53.56

7 moss	
ATOM 943 NH1 ARG 1570	
946 NW2 NDC	5.304 22 22-
A10M 949 C ADC	19.245 6 333
ATOM 950 0 ADO	20.620 1.034 32 222
ATOM 951 N CTT	21.548 0.455 1.00 35.61
ATOM 953 CA CT.	19.677
ATOM 954 CB CI:	19.637 1 955 2. 00 36.79
ATOM 955 CG CIU 15/1	18.403 2.662 24 707
ATOM 956 CD CIV	18.407 4 110 24 1.36
ATOM 957 OF1 CLT	17.048 4 933 24.267 1.00 49.97
ATOM 958 OF2 CHY	15.991 4 133 24.459 1.00 59.14
ATOM 959 C CT	17.043 6.001 24.595 1.00 59.21
ATOM 960 0 CT	19 592 24.446 1.00 59 41
ATOM 961 N 7712	20 327 - 24.948 1.00 37 00
ATOM 963 CD - 1572	18 750 23.892 1.00 37 70
ATOM 964 CD TYR 1572	18 501 24.400 1.00 35 00
ATOM 965 CG TYR 1572	17 571 24.8/8 1.00 30 73
ATOM 966 CT 1YR 1572	17 376 23.995 1.00 31 62
ATTOM 1572	16 302 44.309 1.00 25 60
ATOM: 1572	16 190 - 25.187 1.00 27 92
ATOM 1572	18 151 25.458 1.00 28 52
ATOM OTO CE2 TYR 1572	20.131 -4.941 23.703 1 66 22
ATOM CZ TYR 1572	-6.284 23.969 1 00 00
ATOM OF TYR 1572	16.659 24.852 1 00 05
773 C TYR 1572	20.732 -7.985 25.143 1 00 0-
NTON 974 O TYR 1572	2.525 24.871 1 00 2
MON 9/5 N LEU 1573	25.796 1 55 37.57
977 CA LEU 1573	23.812 1 00 75
9/8 CB LEII 1572	23.712 1 00 25
ATOM 979 CG LEU 1573	22.487 -3.018 22.273 1 00 00
980 CD1 LEU 1573	21.033 -3.888 21.198 1.00
981 CD2 LEU 1573	-3.448 19.840 1 00 75
982 C TETT	-5.354 21 40
983 0 7577	-2.417 24 655
ATOM 984 N Gray	23.752 -3.134 35 333
ATOM 986 CA CIN	23.003 -1.090 24 72-
ATOM 987 CB CIN 175	23.942 -0.399 35 500
ATOM 988 CG CTV	23.844 1.110 25 304
ATOM 989 CD GIN 15-	24.526 1 500 36.96
990 OE1 GLN 1574	24.289 3.054 3.00 39.10
991 NE2 CIN	23.697 3.796 24.502 1.00 40.63
ATOM 994 C CTN	24.736 3.480 33 480
ATOM 995 O GT33	23.687 -0.759 37 075
A10M 996 N 272	24.600 -1.144 27 000
ATOM 998 CA ALA 1575	22.422 -0.731 27 460
ATOM 999 CB ALA 1575	22.021 -1.044 28 833
ATOM 1000 C ALA 1575	20.551 -0.714 20 024
ATOM 1001 O ALA 1575	22.304 -2.484 30 375
ATOM 1000 1	22.006 -2.842 -275 1.00 40.89
ATOM 1004 Ch ARG 1576	22.857 -3 212 30.417 1.00 44.53
ATOM 1005 00	23.148 -4 702 28.395 1.00 39.11
ATOM 1006 CG ARG 1576	2.234 -5 660 -8 1.00 38.24
ATOM 1007 CB ARG 1576 2	0 794 = - 48.019 1.00 38 42
-00/ CD APG 1536	9.838 -6.350 28.472 1.00 39.73
	9.838 -6.352 27.687 1.00 37.87
SSSD/55145 v01	

**ATOM** 1008 NE ARG 1576 18.489 -6.260 28.235 1.00 41.03 ATOM 1010 CZARG 1576 17.830 -5.123 28.436 1.00 43.27 **ATOM** -3.961 1011 NH1 ARG 1576 18.399 28.143 1.00 42.64 **ATOM** 1014 NH2 ARG 1576 16.573 -5.152 28.877 1.00 46.13 **ATOM** 1017 C ARG 1576 24.604 -5.076 28.612 1.00 39.77 **ATOM** 1018 0 ARG 1576 24.978 -6.256 28.623 1.00 40.25 **ATOM** 1019 N ARG 1577 25.428 -4.042 28.501 1.00 40.39 MOTA 1021 CA ARG 1577 26.866 -4.194 28.388 1.00 40.42 MOTA 1022 CB ARG 1577 27.485 -2.871 27.952 1.00 37.67 MOTA 1023 CG ARG 1577 27.247 -2.477 26.526 1.00 36.22 ATOM 1024 CD ARG 1577 27.857 -1.113 26.287 1.00 35.55 **ATOM** 1025 NE ARG 1577 27.971 -0.797 24.866 1.00 38.72 MOTA 1027 CZARG 1577 28.395 0.369 24.384 1.00 37.57 MOTA 1028 NH1 ARG 1577 28.754 1.352 25.205 1.00 37.49 MOTA 1031 NH2 ARG 1577 28.449 0.562 23.074 1.00 39.58 **ATOM** 1034 C ARG 1577 27.449 -4.548 29.760 1.00 42.45 **ATOM** 1035 0 ARG 1577 26.878 -4.180 30.801 1.00 42.57 **ATOM** 1036 N PRO 1578 28.564 -5.296 29.797 1.00 43.36 ATOM 1037 CD PRO 1578 29.270 -5.985 28.692 1.00 42.43 ATOM 1038 CA PRO 1578 29.159 -5.648 31.082 1.00 43.08 ATOM 1039 CB PRO 1578 30.225 -6.676 30.709 1.00 40.33 ATOM 1040 CG PRO 1578 30.600 -6.300 29.331 1.00 40.71 ATOM 1041 С -4.373 PRO 1578 29.768 31.666 1.00 42.44 **ATOM** 1042 PRO 0 1578 30.261 -3.525 30.922 1.00 41.24 ATOM 1043 N PRO 1579 29.705 -4.205 32.993 1.00 44.57 **ATOM** 1044 CD PRO 1579 29.169 -5.143 33.994 1.00 46.68 ATOM 1045 CA PRO 1579 30.251 -3.017 33.654 1.00 44.89 ATOM 1046 PRO CB 1579 30.088 -3.356 35.134 1.00 45.31 MOTA 1047 CG PRO 1579 28.865 -4.224 35.142 1.00 44.45 **ATOM** 1048 C PRO 1579 31.711 -2.767 33.289 1.09 45.17 **ATOM** 1049 PRO 0 1579 32.620 -3.257 33.953 1.00 47.72 **ATOM** 1050 N ALA 1592 19.075 -5.384 32.475 1.00 49.23 MOTA 1052 CA ALA 1592 20.500 -5.078 32.354 1.00 50.33 **ATOM** 1053 CB ALA 1592 20.954 -4.184 33.503 1.00 51.83 **ATOM** 1054 C ALA 1592 21.412 -6.308 32.251 1.00 50.65 **ATOM** 1055 0 ALA 1592 22.621 -6.166 32.044 1.00 51.55 ATOM 1056 N ALA 1593 20.849 -7.505 32.409 1.00 49.06 ATOM 1058 CA ALA 1593 21.638 -8.735 32.294 1.00 48.07 ATOM 1059 CB ALA 1593 20.773 -9.953 32.579 1.00 47.87 **ATOM** 1060 C ALA 1593 22.258 -8.840 30.891 1.00 47.59 **ATOM** 1061 0 ALA 1593 21.664 -8.426 29.894 1.00 49.09 **ATOM** 1062 N GLN 1594 23.465 -9.388 30.830 1.00 47.30 ATOM 1064 GLN CA 1594 24.186 -9.553 29.569 1.00 45.32 ATOM 1065 CB GLN 1594 25.576 -10.118 29.837 1.00 44.82 **ATOM** 1066 CG GLN 1594 26.523 -9.166 30.542 1.00 49.34 MOTA 1067 CD GLN 1594 27.751 -9.877 31.111 1.00 52.40 **ATOM** 1068 OE1 GLN 1594 28.264 -10.847 30.537 1.00 51.16 MOTA 1069 NE2 GLN 1594 32.265 28.209 -9.408 1.00 54.00 **ATOM** 1072 C GLN 1594 23.474 -10.432 28.539 1.00 45.00 ATOM 1073 0 GLN 1594 22.780 -11.393 28.876 1.00 45.28 MOTA 1074 N LEU 1595 23.684 -10.104 27.273 1.00 45.08 **ATOM** 1076 CA LEU 1595 23.084 -10.828 26.169 1.00 44.65

	ma	1077		LEU	1595	22 760
	TOM	1078	CG	LEU	1595	22.738 -9.864 25.023 1.00 43 05
		1079	CD1	LEU	1595	25.295 1 00 42 20
		1080	CD2	LEU	1595	7.303 24.564 1 00 41 75
	TOM ]	1801	C	LEU	1595	20.2/6 -9.510 24.918 1 00 45
	TOM 1	082	0	LEU	1595	24.044 -11.885 25 605 3
		083	N	SER	1596	23.252 ~11.661 25 622
	COM 1	085	CA		1596	23.311 -13.058 25 376
	OM 1	086	CB		1596	24.325 -14.151 24 969 3 3
	OM 1	087	OG		1596	23.633 -15.495 25 124
AT		089	_			22.401 -15.605 24 422 -
AT		090	_		1596	24.557 -13.968 23 366 3 3
ATO		91			1596	23.891 -13.156 22 707 3 3
ATO	^	93	`		1597	25.475 -14.756 22 922 1 -2
ATC		194			.597	25.782 -14.690 21 407
ATC		95			597	26.921 -15 643
ATO		97			597	27.976 -15 516 -100 45.60
ATO	M 10				597	24.526 -15.036
ATO				_	597	24.233 -14 400
ATO		~ -			598	23.767 -16 025 11.00 45.51
ATO		_			598	22.551 -16 4-4
ATO	M 110				598	21.978 - 17.736 1.00 36.56
ATON					598	21.374 - 10 (42 1.00 34.93
ATON					98	20.450 -19 665 -1.00 37.52
ATOM			E L		98	20.054 20 20 34.85
ATOM		_	IZ LY	_	98	21.219 -21 55
ATOM					98	21.521 15 226 100 30.59
ATOM		_			98 .	20.840 - 15.000 1.00 36.21
ATOM		_			99	21.447 -14 624
ATOM					99	20.520 -13 500 21.681 1.00 33.57
ATOM		_			99	20.635 -12 000
ATOM		_			99	20.143 -13 000
ATOM	1117		D1 AS			20,659 13 27 1.00 38.08
ATOM	1118 1119		02 AS1		9	19.256 -14 601 - 1.00 37.52
ATOM			ASI		9	20.777 -12 470 24.072 1.00 36.17
ATOM	1120	_	ASI			19.846 -17.045 -1.00 30.89
ATOM	1121		LEU			22.046 -12.020 20.153 1.00 30.88
ATOM	1123	CA		160	0	22.439 -11 050 20.636 1.00 31.39
ATOM	1124	CB				23.921 -10.605
ATOM	1125	CG			0	24.341 -10.000 19.845 1.00 30.47
ATOM	1126		1 LEU	1600	)	25 057 21.190 1.00 29.24
ATOM	1127	CD:	2 LEU	1600	)	23 666 0 771 21.226 1.00 29.75
ATOM	1128	C	LEU	1600	)	22 126
ATOM	1129	0	LEU	1600	)	21 620 18.212 1.00 31 39
ATOM	1130	N	VAL	1601		22 422
	1132	CA	VAL	1601		22 161 17.863 1.00 30.00
ATOM	1133	CB	VAL	1601		22 027 16.518 1.00 27 94
ATOM	1134	CG1	VAL	1601		22 467 - 16.261 1.00 27.68
ATOM	1135	CG2	VAL	1601		24 335 1.00 24 69
ATOM	1136	C	VAL	1601		20 (42 16.362 1.00 25.87
ATOM	1137	0	VAL	1601		20.642 -13.340 16.310 1.00 28 98
ATOM	1138	N	SER	1602		20.152 -13.151 15.191 1.00 28 55
ATOM	1140	CA	SER	1602		19.904 -13.635 17 202
			-			18.450 -13.726 17.318 1.00 27.64 17.318 1.00 27.07
SSCD/Free						-100 27.07



MOTA	1141	CB	SER	1602	17.899 -14.362	18.584	1.00 29.97
ATOM	1142	QG	SER	1602	16.488 -14.202	18.673	1.00 38.86
MOTA	1144	С	SER	1602	17.864 -12.327	17.093	1.00 27.45
ATOM	1145	0	SER	1602	16.826 -12.181	16.438	1.00 29.38
ATOM	1146	N	CYS	1603	18.504 11.306	17.663	1.00 25.31
ATOM	1148	CA	CYS	1603	18.087 -9.909	17.461	1.00 24.49
MOTA	1149	CB	CYS	1603	19.074 -8.965	18.143	1.00 21.15
MOTA	1150	SG	CYS	1603	18.716 -7.213	18.030	0.50 11.83 PRT1
ATOM	1151	С	CYS	1603	18.155 -9.628	15.961	1.00 26.92
ATOM	1152	0	CYS	1603	17.175 -9.238	15.329	1.00 30.04
ATOM	1153	N	ALA	1604	19.340 -9.833	15.398	1.00 28.35
ATOM	1155	CA	ALA	1604	19.573 -9.611	13.979	1.00 28.00
ATOM	1156	CB	ALA	1604	20.970 10.098	13.588	1.00 25.49
ATOM	1157	C	ALA	1604	18.517 -10.295	13.132	1.00 26.69
ATOM	1158	0	ALA	1604	17.892 -9.646	12.310	1.00 31.40
MOTA	1159	N	TYR	1605	18.270 -11.577	13.399	1.00 26.33
ATOM	1161	CA	TYR	1605	17.286 -12.384	12.666	1.00 24.79
ATOM	1162	CB	TYR	1605	17.209 -13.771	13.300	1.00 23.42
ATOM	1163	CG	TYR	1605	16.132 -14.663	12.742	1.00 29.93
MOTA	1164		TYR	1605	16.281 - 15.298	11.510	1.00 30.00
ATOM	1165	CE1		1605	15.270 -16.097	10.989	1.00 32.29
ATOM	1166	CD2		1605	14.949 -14.859	13.441	1.00 32.69
ATOM	1167		TYR	1605	13.935 -15.650	12.934	1.00 33.02
ATOM	1168	CZ	TYR	1605	14.091 -16.266	11.713	1.00 34.40
A'TOM	1169	OH	TYR	1605	13.037 -17.023	11.225	1.00 34.18
ATOM	1171	C	TYR	1605	15.885 -11.750	12.572	1.00 26.08
ATOM	1172	C	TYR	1605	15.327 -11.587	11.475	1.00 25.43
ATOM ·	1173	N	GLN	1606	15.337 -11.366	13.717	1.00 25.38
ATOM	1175	CA	GLN	1606	14.018 -10.737	13.776	1.00 25.47
ATOM	1176	CB	GLN	1606	13.662 -10.424	15.227	1.00 24.21
ATOM ATOM	1177	CG	GLN	1606	13.642 -11.636	16.127	1.00 24.37
ATOM	1178 1179	CD	GLN	1606	13.237 -11.279	17.540	1.00 27.16
ATOM			GLN	1606	12.227 -10.603	17.758	1.00 29.64
ATOM	1180		GLN	1606	14.033 -11.705	18.507	1.00 30.69
ATOM	1183 1184	0	GLN	1606	13.953 -9.449	12.949	1.00 26.89
ATOM	1185	N	GLN VAL	1606 1607	12.936 -9.136	12.319	1.00 26.40
ATOM	1187	CA	VAL	1607	15.030 -8.674 15.120 -7.430	13.000	1.00 27.79
ATOM	1188	CB	VAL	1607	15.120 -7.430 16.408 -6.667	12.255 12.625	1.00 26.35
ATOM	1189		VAL	1607	16.556 -5.433	11.752	1.00 24.87 1.00 25.90
ATOM	1190		VAL	1607	16.382 -6.282	14.094	1.00 23.90
ATOM	1191	C	VAL	1607	15.121 -7.743	10.757	1.00 17.95
ATOM	1192	0	VAL	1607	14.406 -7.093		1.00 27.69
ATOM	1193	N	ALA	1608	15.902 -8.749	9.979	
ATOM	1195	CA	ALA	1608	15.965 -9.135	10.355	1.00 24.59
ATOM	1196	CB	ALA	1608	16.971 -10.227	8.950 8.750	1.00 23.22 1.00 17.65
ATOM	1197	C	ALA	1608	14.579 -9.589	8.492	1.00 17.65
ATOM	1198	Ō	ALA	1608	14.201 -9.372	7.337	1.00 24.58
ATOM	1199	N	ARG	1609	13.819 -10.191	9.409	1.00 26.22
ATOM	1201	CA	ARG	1609	12.453 -10.648	9.124	1.00 25.65
ATOM	1202	CB	ARG	1609	11.998 -11.660	10.160	1.00 24.86
ATOM	1203	CG	ARG	1609	12.451 -13.050	9.863	1.00 28.15
					12.431 -13.030	3.003	1.00 30.10

* mov	
ATOM 1204 CD ARG 1609	7.2
ATOM 1205 NE ARG 1600	11.683 -13.980 10.723 1.00 32.49
ATOM 1207 CZ ARG 1600	10.942 -14.941 9 927
ATOM 1200	10.058 -15.792 10 437 1 22
ATOM 1311	9.800 -15 700
ATOM 1214 C	9.468 -16 670 - 1.00 32.47
ATOM 1215 0 ARG 1609	11.421 -9 510 - 1.00 36.67
ATOM 1216 " ARG 1609	10.5229 500
ATOM 1222	11 501 8.155 1.00 23.65
ATOM 1218 CA GLY 1610	10 501 7 9.888 1.00 20.88
1219 C GLY 1610	7.338 9.789 1 00 31 45
110M 1220 O GLY 1610	8.432 1 00 22 55
ATOM 1221 N MET 1611	9.8/2 -6.452 7.600
ATOM 1223 CD	12.097 -6.558 8 000 1 as
ATOM 1224 TOTI	12.488 -5.955 6 800
ATOM 1225 00 1151	13.991
ATOM 1226	14.391 -4 470
ATOM 1337 05 MET 1611	13.362 -3.000 7.652 1.00 27.09
ATOM LE MET 1611	13 665 2.500 7.330 1.00 22.57
MET 1611	12 000 5.612 1.00 21 91
OM 1229 O MET 1611	5.590 1 00 26 57
1230 N GLU 1612	4.553 1 00 24 00
ATOM 1232 CA GLU 1612	12.213 8.108 5.710 1.00 37.75
ATOM 1233 CB GLU 1612	4.632 1.00 05
ATOM 1234 CG GUI 1600	12.120 -10.446 5 024 7 05
ATOM 1235 CD GITT 1630	11.602 -11.443 4 036
ATOM 1236 OF1 CIV 1512	11.796 -12.872 4 477 1 20
ATOM 1237 OF 5	11.658 -12 442
ATOM 1238 C	12.085 -13
ATOM 1220 " GLU 1612	10.354 - 0.12
ATOM 1010 1612	9.974 - 9.665 4.305 1.00 27.55
ATOM 1215	9.570 3.130 1.00 30.04
ATOM 1218 1613	9 000 5.732 5.337 1.00 25 11
CB TYR 1613	7 343 5.133 1.00 21 91
1 IK 1613	- 5.025 6.462 1 00 21 00
1245 CD1 TYR 1613	0.310 0.335 1 00 15
1246 CE1 TYR 1613	4.969 -9.307 5.968 1 00 10 3
ATOM 1247 CD2 TYR 1613	3.610 -9.049 5.872 1 00 10 00
ATOM 1248 CE2 TVP 1612	5.373 -7.041 6.600 1.00 -
ATOM 1249 CZ TVP 1513	4.017 -6.761 6.502
ATOM 1250 OT	3.137 -7.776
ATOM 1252 C	1.779 -7 543
ATOM 1252 - TO 13	7 870 7 21.91
ATOM 1254	7.125 7.02
ATOM 1356 55	8 541 6 10 3 3 3 3 4 0 1 0 0 22 01
ATOM 1355	8,400 4 724 5.045 1.00 22.04
ATOM 1614	4.536 1.00 20.56
Amose 1614	9.540 5.392 1.00 18.43
A10M 1259 CD1 LEU 1614	6.707 1 00 15 06
ATOM 1260 CD2 LEU 1614	2.5/1 /.518 1 00 15 70
ATOM 1261 C LEU 1614	7.255 -2.647 6.436 1.00 13.06
ATOM 1262 O LEU 1614	8.793 -4.671 3.066 1.00 22 62
ATOM 1262 V	8.156 -3.939 2 294 7 20
ATOM 1265 CA ALA 1615	9.840 -5.397 2.684 1.55
ATOM 1266 CB NIA 1615	10.333 -5.408 1 317 1 22
ATOM 1267 C	11.685 -6 000 21.18
1267 C ALA 1615	9 334 6 10- 1.234 1.00 18.35
	9.334 -6.107 0.404 1.00 21.97
CCCP	

ATOM	1268	0	ALA	1615	9.089	-5.642	-0.705	1.00 23.80
ATOM	1269	N	SER	1616	8.704	-7.173	0.893	1.00 22.49
MOTA	1271	CA	SER	1616	7.722	-7.919	0.097	1.00 21.81
MOTA	1272	CB	SER	1616	7.305	-9.179	0.831	1.00 19.78
ATOM	1273	OG	SER	1616	6.382	-8.862	1.851	1.00 23.88
MOTA	1275	C	SER	1616	6.475	-7.071	-0.149	1.00 23.60
ATOM	1276	0	SER	1616	5.733	-7.277	-1.117	1.00 21.74
MOTA	1277	N	LYS	1617	6.217	-6.169	0.789	1.00 25.84
ATOM	1279	CA	LYS	1617	5.078	-5.280	0.705	1.00 23.96
ATOM	1280	CB	LYS	1617	4.555	-4.951	2.099	1.00 20.74
ATOM	1281	CG	LYS	1617	3.843	-6.124	2.750	1.00 23.40
MOTA	1282	CD	LYS	1617	2.509	-6.395	2.081	1.00 28.70
MOTA	1283	CE	LYS	1617	1.714	-7.442	2.809	1.00 31.16
ATOM	1284	NZ	LYS	1617	2.339	-8.767	2.616	1.00 41.91
MOTA	1288	С	LYS	1617	5.409	-4.019	-0.061	1.00 24.25
MOTA	1289	Ō	LYS	1617	4.640	-3.053	-0.022	1.00 25.22
MOTA	1290	N	LYS	1618	6.557	-4.028	-0.748	1.00 24.20
MOTA	1292	CA	LYS	1618	7.014	-2.904	-1.582	1.00 25.15
ATOM	1293	CB	LYS	1618	5.906	-2.507	-2.571	1.00 27.00
ATOM	1294	CG	LYS	1618	5.735	-3.411	-3.790	1.00 29.09
.ATOM	1295	CD	LYS	1618	5.506	-4.864	3.432	1.00 31.82
ATOM	1296	CE	LYS	1618	5.533	-5.752	-4.663	1.00 30.21
ATOM	1297	NZ	LYS	1618	4.231	-5.707	-5.369	1.00 26.34
MOTA	1301	C	LYS	1618	7.466	-1.658	-0.816	1.00 23.50
ATOM	i302	0	LYS	1618	7.537	-0.576	-1.385	1.00 22.10
ATOM	1.303	N	CYS	1619	7.827	-1.821	0.449	1.00 23.72
ATOM	1305	CA	CYS	1619	8.213	-0.693	1.276	1.00 20.89
ATOM	1306	CB	CYS	1619	7.535	-0.814	2.647	1.00 18.41
ATOM	1307	SG	CYS	1619	8.019	0.405	3.894	1.00 26.34
ATOM	1308	С	CYS	1619	9.717	-0.529	1.451	1.00 22.94
ATOM	1309	0	CYS	1619	10.419	-1.487	1.790	1.00 23.20
MOTA	1310	M	ILE	1620	10.197	0.690	1.211	1.00 21.17
ATOM	1312	CA	ILE	1620	11.610	1.039	1.388	1.00 22.35
ATOM	1313	CB	ILE	1620	12.151	1.823	0.172	1.00 17.30
ATOM	1314	CG2	ILE	1620	13.607	2.215	0.393	1.00 8.27
ATOM	1315	CG1	ILE	1620	11.966	0.997	-1.111	1.00 18.27
MOTA	1316	CD1	ILE	1620	12.127	1.803	-2.401	1.00 17.57
MOTA	1317	C	ILE	1620	11.631	1.926	2.652	1.00 25.20
MOTA	1318	O	ILE	1620	10.912	2.932	2.715	1.00 29.69
ATOM	1319	N	HIS	1621	12.398	1.526	3.665	1.00 22.66
ATOM	1321	CA	HIS	1621	12.463	2.254	4.931	1.00 22.78
MOTA	1322	CB	HIS	1621	13.214	1.425	5.980	1.00 22.65
ATOM	1323	CG	HIS	1621	13.024	1.897	7.398	1.00 22.07
ATOM	1324	CD2	HIS	1621	12.485	1.280	8.475	1.00 20.50
ATOM	1325	ND1		1621	13.449	3.134	7.842	1.00 23.11
ATOM	1327	CEI		1621	13.182	3.253	9.131	1.00 23.92
ATOM	1328	NE2		1621	12.596	2.144	9.543	1.00 24.44
ATOM	1330	C	HIS	1621	13.110	3.616	4.831	1.00 24.07
ATOM	1331	0	HIS	1621	12.561	4.597	5.306	1.00 24.37
ATOM	1332	N	ARG	1622	14.327	3.639	4.291	1.00 26.42
ATOM	1334	CA	ARG	1622	15.129	4.853	4.130	1.00 24.59
ATOM	1335	CB	ARG	1622	14.289	6.018	3.581	1.00 17.58
					-1.203	2.010	5.501	UU 1/.JO

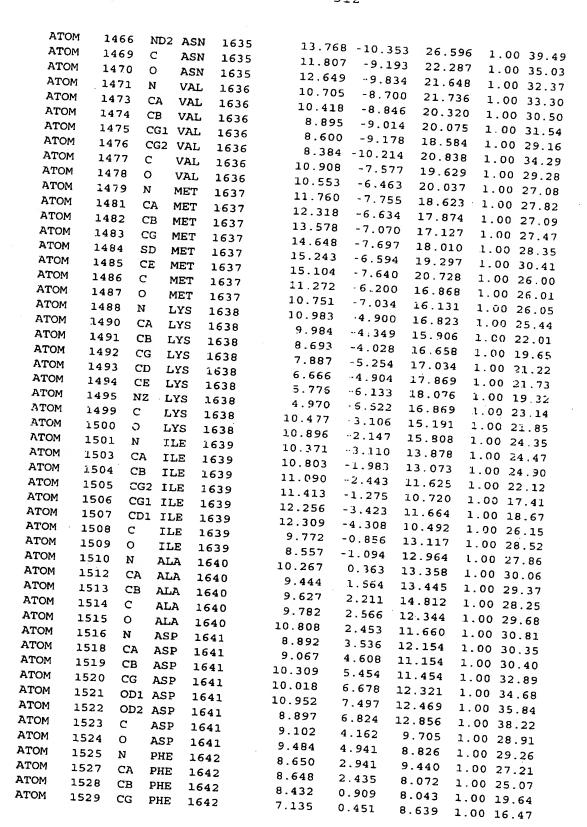
Δ.	TOM 1										
		.336	CG	ARG	1622	13.8	110 -	7			
		337	CD	ARG	1622	12.9			.163	1.00	13.88
		338	NE	ARG	1622				.634	0.50	4.97
		340	CZ	ARG	1622	12.5		.590 0	. 243	0.50	6.49
	OM 1	341	NH1		1622	11.5		852 -0	. 145	0.50	3.84
	'OM 1:	344	NH2			10.7			753	0.50	
	OM 1:	347	_	ARG	1622	11.3			433	0.50	2.25
AT		348	_	ARG	1622	15.9	L8 5.		388		2.48
AT		349			1622	16.76			337	1.00	24.72
AT	~	51		ASP	1623	15.68		•	505	1.00	26.90
ATO	~	52		ASP	1623	16.43				1.00	25.61
ATO		53	_	ASP	1623	15.92			703	1.00	28.41
ATO	-			ASP	1623	16.89			349	1.00	30.38
ATO			OD1	ASP	1623	16.42			373	1.00 3	33.47
ATO				ASP	1623	18.12	_		382	1.00 4	13.35
			C I	SP	1623	16.49	_		.67	1.00 3	1.88
ATO			O A	SP	1623	16.14			13 ;	1.00 2	8.86
ATO			N L		1624	10.14	-		87 ]	1.00 2	8 31
ATO		50	CA L		1624	16.956			46 1	.00 2	7 01
ATO		1	_		1624	17.087	-	80 <u>9.1</u>		.00 2	7.01
OTA	M 136	2 (			1624	17.149		20 8.2	42 1	.00 2	7.28
ATOM	<sup>4</sup> 136		D1 L			17.118		50 8.9		.00 2	7.53
ATON	1 136		D2 L		1624	15.850	-1.34	18 9.7	_	.00 2	7.69
ATOM	1 136				1624	17.228	-2.17			.00 23	3.77
ATOM	1 136	_			L624	18.340	1.62		_	.00 29	9.15
ATOM		-		-	624	19.464	1.77			.00 26	5.27
ATOM			-	-	.625	18.116	1.59			.00 25	.89
ATOM			A AL	_	625	19.164	1.75			.00 23	.29
ATOM					625	19.520	3.23			00 19	.68
ATOM	-5,3				625	18.575	1.21			00 18	.85
ATOM		_	AL	A 1	625	17.352				00 20	. 79
ATOM	1373		AL.	A L	626	19.429	1.07			00 20	. 75
	1375			A 16	526	18.969	0.942		51.	00 22	. 03
ATOM	1376		3 AL		526	20.139	0.408		0 1.	00 23	. 43
ATOM	1377	_	AL		526	18.111	-0.048		1 1.	00 22,	46
ATOM	1378		ALA		26		1.397		1.	00 25.	86
ATOM	1379	N	ARG		27	17.333	1.006		1.0	00 29.	51
MOTA	1381	CA			27	18.303	2.685		· 1.0	0 26.	92
ATOM	1382	CB			27	17.503	3.722	17.048		0 27.	30
ATOM	1383	CG				18.017	5.107	16.627		0 28.	30
ATOM	1384	CD	ARG			18.086	5.287	15.104		0 36.	29
ATOM	1385	NE	ARG			18.255	6.756	14.688		0 41.	
ATOM	1387	CZ		16:		18.548	6.928	13.261			
ATOM	1388		ARG ARG	16:		19.779	6.904	12.749	1.0	0 39.	94
ATOM	1391			162		20.826	6.721	13.539	1.0	0 42.3	33
ATOM	1394		ARG	162		19.976	7.059	11.450	1.0	0 44.7	75
ATOM		C	ARG	162		16.029	3.567		1.0	0 41.5	50
ATOM	1395	0	ARG	162		15.092	3.897	16.591	1.0	27.4	2
ATOM	1396	N	ASN	162		15.850	3.039	17.333	1.00	26.5	3
	1398	CA	ASN	162	8	14.534		15.375	1.00	26.8	2
ATOM	1399	CB	ASN	162		14.569	2.849	14.758	1.00	24.0	8
ATOM	1400	CG	ASN	162		14.709	3.308	13.301	1.00	26.3	0
ATOM	1401	OD1	ASN	162			4.823	13.167	1.00	25.1	9
ATOM	1402		ASN	162		14.018	5.567	13.844	1.00	28.5	9
ATOM	1405	C	ASN	1628			5.277	12.297	1.00	22.3	-
				-940	-	13.945	1.440	14.862	1.00	24.35	
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ATOM	1406	0	ASN	1628	13.026	1.084	14.105	1.00 24.66
ATOM	1407	N	VAL	1629	14.473	0.637	15.785	1.00 22.35
ATOM	1409	CA	VAL	1629	13.988	-0.718	16.055	1.00 20.65
ATOM	1410	CB	VAL	1629	15.077	-1.813	15.822	1.00 18.07
ATOM	1411	CG1	VAL	1629	14.612	-3.142	16.398	1.00 11.84
ATOM	1412	CG2	VAL	1629	15.378	-1.977	14.346	1.00 12.65
MOTA	1413	С	VAL	1629	13.625	-0.670	17.536	1.00 24.27
MOTA	1414	0	VAL	1629	14.427	-0.237	18.361	1.00 25.94
ATOM	1415	N	LEU	1630	12.393	-1.031	17.866	1.00 24.99
ATOM	1417	CA	LEU	1630	11.936	-1.010	19.247	1.00 25.50
MOTA	1418	CB	LEU	1630	10.609	-0.252	19.339	1.00 22.79
MOTA	1419	CG	LEU	1630	10.634	1.179	18.789	1.00 17.86
MOTA	1420	CD1	LEU	1630	9.240	1 680	18.654	1.00 18.49
.ATOM	1421	CD2	LEU	1630	11.409	2.100	19.668	1.00 17.63
MOTA	1422	C	LEU	1630	11.833	-2.434	19.829	1.00 28.29
MOTA	1423	0	LEU	1630	11.666	-3.412	19.092	1.00 28.56
ATOM	1424	N	VAL	1631	11.933	-2.542	21.150	1.00 29.46
ATOM	1426	CA	VAL	1631	11.883	-3.831	21.833	1.00 29.40
MOTA	1427	CB	VAL	1631	13.222	-4.105	22.553	1.00 27.48
ATOM	1428	CG1	VAL	1631	13.210	-5.477	23.233	1.00 24.53
MOTA	1429	CG2	VAL	1631	14.376	-3.976	21.576	1.00 22.55
ATOM	1430	С	VAL	1631	10.730	-3.918	22.853	1.00 31.94
ATOM	1431	0	VAL	1631	10.630	-3.102	23.787	1.00 33.13
ATOM	1432	N	THR	1632	9.866	.4.911	22.659	1.00 32.21
ATOM	1434	CA	'THR	1632	8.728	-5.149	23.540	1.00 31.77
ATOM	1435	CB	THR	1632	7.674	6.061	22.374	1.00 32.38
ATOM	1436	OG1	THR	1632	8.169	-7.406	22.792	1.00 32.38
ATOM	1438	CG2	THR	1632	7.330	5.554	21.480	1.00 28.05
ATOM	1439	C	THR	1632	9.157	-5.810	24.842	1.00 30.39
ATOM	1440	O	THR	1632	10.256	-6.320	24.947	1.00 30.28
ATOM	1441	N	GLU	1633	8.260	-5.823	25.822	1.00 32.43
ATOM	1443	CA	GLU	1633	8.513	-6.424	27.122	1.00 32.84
ATOM	3.444	CB	GLU	1633	7.259	-6.310	27.991	1.00 35.28
MOTA	1.445	CG	GLU	1633	7.386	-6.881	29.399	1.00 46.57
ATOM	1446	CD	GLU	1633	8.463	-6.192	30.260	1.00 54.03
ATOM	1447	OE1	GLU	1633	8.519	-4.939	30.297	1.00 58.68
MOTA	1448	OE2	GLU	1633	9.249	-6.916	30.918	1.00 56.84
ATOM	1449	C	GLU	1633	8.914	-7.889	26.986	1.00 35.14
MOTA	1450	0	GLU	1633	9.632	-8.435	27.826	1.00 33.92
ATOM	1451	N	ASP	1634	8.456	-8.526	25.910	1.00 38.25
ATOM	1453	CA	ASP	1634	8.768	-9.941	25.677	1.00 39.22
ATOM	1454	CB	ASP	1634		-10.639	24.990	1.00 44.88
ATOM	1455	CG	ASP	1634	6.258	-10.420	25.725	1.00 54.17
MOTA	1456	OD1		1634		-11.042	26.799	1.00 56.33
ATOM	1457	OD2		1634	5.412	-9.622	25.236	1.00 54.47
MOTA	1458	С	ASP	1634		-10.109	24.849	1.00 37.53
ATOM	1459	ō	ASP	1634		-11.225	24.495	1.00 36.33
MOTA	1460	N	ASN	1635	10.730	-8.998	24.589	1.00 39.12
ATOM	1462	CA	ASN	1635	11.974	-8.948	23.792	1.00 37.21
ATOM	1463	CB	ASN	1635	13.042	-9.891	24.361	1.00 37.83
ATOM	1464	CG	ASN	1635	13.576	-9.426	25.677	1.00 38.65
ATOM	1465	OD1		1635	13.795	-8.236	25.880	1.00 43.82



MOTA	1530	CD1	L PHE	1642	5.974	0.400	7.878	1.00	21.72
ATOM	1531	CD2	PHE	1642	7.080	0.018	9.945	1.00	17.01
MOTA	1532	CE	L PHE	1642	4.781	-0.082	8.422	1.00	20.97
ATOM	1533	CE2	PHE	1642	5.892	-0.463	10.496	1.00	18.72
MOTA	1534	CZ	PHE	1642	4.743	-0.515	9.739	1.00	20.32
ATOM	1535	С	PHE	1642	7.667	3.174	7.157	1.00	25.57
ATOM	1536	0	PHE	1642	7.910	3.292	5.971	1.00	28.40
ATOM	1537	N	GLY	1643	6.585	3.718	7.707	1.00	25.69
ATOM	1539	CA	GLY	1643	5.631	4.427	6.866	1.00	24.81
MOTA	1540	C	GLY	1643	5.786	5.935	6.893		24.84
ATOM	1541	0	GLY	1643	4.922	6.684	6.436	1.00	19.20
ATOM	1542	N	LEU	1644	6.930	6.387	7.376	1.00	29.50
MOTA	1544	CA	LEU	1644	7.189	7.808	7.491		34.24
ATOM	1545	CB	· LEU	1644	8.498	8.037	8.242		33.10
ATOM	1546	ÇG	LEU	1644	8.473	9.371	8.962		36.00
ATOM	1547	CD1	LEU	1644	7.520	9.212	10.127		41.52
ATOM	1548	CD2	LEU	1644	9.854	9.773	9.442		35.23
ATOM	1549	С	LEU	1644	7.213	8.578	6.179	1.00	
MOTA	1550	0	LEU	1644	7.759	8.123	5.176	1.00	
ATOM	1551	N	ALA	1645	6.577	9.744	6.203		41.66
ATOM	1553	CA	ALA	1645	6.524	10.652	5.067	1.00	
ATOM	1554	CB	ALA	1645	5.309	11.563	5.202	1.00	38.13
ATOM	1555	C	ALA	1645	7.819	11.475	5.141	1.00	
ATOM	1556	0	ALA	1645	8.105	12.082	6.176	1.00	47.17
ATOM	1557	Ŋ	ALA	1646	8.622	11.462	4.082	1.00	45.69
ATOM	1559	CA	ALA	1646	9.871	12.222	4.094		48.62
ATOM	1560	CB	ALA	1646	10.971	11.405	4.778	1.00	49 50
MOTA	1561	C	ALA	1646	10.338	12.661	2.712	1.00	50.98
MOTA	1562	0	ALA	1646	10.319	11.880	1.759	1.00	52.84
ATOM	1563	N	ASP	1647	10.755	13.919	2.598	1.00	53.09
MOTA	1565	CA	ASP	1647	11.253	14.419	1.322	1.00	55.06
ATOM	1566	CB	ASP	1647	10.868	15.887	1.092	1.00	56.05
MOTA	1567	CG	ASP	1647	11.084	16.342	-0.352	1.00	59.31
ATOM	1568	OD1	ASP	1647	12.070	15.928	-1.003	1.00	59.51
ATOM	1569	OD2	ASP	1647	10.265	17.150	-0.837	1.00	63.48
MOTA	1570	C	ASP	1647	12.770	14.264	1.332	1.00	55.26
MOTA	1571	0	ASP	1647	13.487	15.075	1.926	1.00	53.18
ATOM	1572	N	ILE	1648	13.235	13.198	0.684	1.00	56.66
MOTA	1574	CA	ILE	1648	14.652	12.877	0.595	1.00	57.79
ATOM	1575	CB	ILE	1648	14.890	11.624	-0.271	1.00	53.86
ATOM	1576	CG2		1648	14.133	10.443	0.326	1.00	52.14
ATOM	1577		ILE	1648	14.454	11.886	-1.718	1.00	48.24
MOTA	1578	CD1	ILE	1648	15.198	11.083	-2.751	1.00	43.97
ATOM	1579	C	ILE	1648	15.439	14.044	0.014	1.00	62.32
MOTA	1580	0	ILE	1648	16.591	14.271	0.380	1.00	64.72
MOTA	1581	N	HIS	1649	14.805	14.791	-0.884	1.00	65.72
ATOM	1583	CA	HIS	1649	15.450	15.941	-1.500	1.00	69.00
ATOM	1584	CB	HIS	1649	14.793	16.285	-2.844	1.00	70.35
ATOM	1585	CG	HIS	1649	15.123	15.332	-3.944	1.00	73.90
MOTA	1586	CD2	HIS	1649	16.257	14.628	-4.208	1.00	75.13
ATOM	1587	ND1	HIS	1649	14.239	15.006	-4.946	1.00	75.30
ATOM	1589	CE1	HIS	1649	14.798	14.148	-5.779		76.83



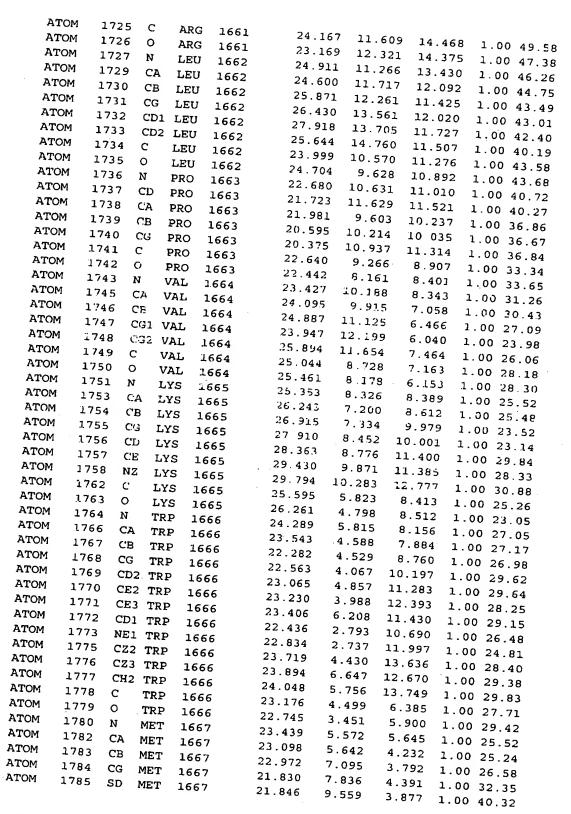
ATOM 1590 NE2 HIS	1640
ATOM 1592 C HIS	1649 16.025 13.905 -5.348 1.00 76 74
ATOM 1593 O HIS	15.419 17.150 -0 576 1 00
ATOM 1594 N HIS	15.517 18 204
ATOM 1505	15.218 16 912 0 72.83
ATOM 1507	15.199 17 007
ATOM 1500	1650 13.776 19.400 1.00 72.52
ATOM 1599 CD2 tras	1650 13.272 19.403 1.936 1.00 75.67
ATOM 1600 NO.	1650 13.451 20 734 0.002 1.00 82.16
ATOM 1600 -	1650 12.529 18 055 1.00 86.17
ATOM 1602	1650 12.262 19.022 0.165 1.00 86.37
ATOM 100	1650 12.814 21.050 0.333 1.00 89.04
ATOM 3505 C HIS	1650 15.856 17.503 =0.481 1.00 89.37
ATOM 150-	1650 15 782 23 3.029 1.00 71.11
ATOM 1500	.651 16.543 25 4.010 1.00 69.56
ATOM NOTE IN	651 17 221 1- 3.033 1.00 70.84
ATOM 1	651 17 600 1.222 1.00 70 50
THOM 1611 CG2 ILE 1	651 14.462 4.031 1.00 71 75
Amous 1612 CG1 ILE 1	651 13.9/8 5.194 1 00 71 62
1613 CD1 ILE 1	651 13.604 3.890 1.00 23 26
1614 C ILE 10	551 3.593 1.00.75 10
1615 O ILE 16	551 4.569 1 00 60 00
1616 N ASP 16	15.3 16.882 3.745 1.00 70 70
1618 CA ASP 16	5.802 7.00 60 65
1619 CB ASP 16	52 6.240 1 00 60 06
Amous 1620 CG ASP 16	52 18.923 7 398 1 00 70 52
1621 OD1 ASP 16	52 7.843 100 72 00
ATOM 1622 OD2 ASP 16	52 20.248 b. 985 1 00 73 36
ATOM 1623 C ASD 16	52 20.646 20.034 9.060 1.00 76 05
1624 O ASP 160	52 20.802 17.023 5.673 1 00 66 00
ATOM 1625 N TVD 16	20.746 16.457 7.762 1.00 (4.00
1627 CA TVD 36.	12 16.856 5.814 1 00 54.72
ATOM 1628 CR TVD	22.926 15.968 6.089 1.00 63.00
ATOM 1629 CG TVD 165	23.852 15.906 4.875 1.00.61.20
ATOM 1630 CD1 TYR 165	3 23.362 14.971 3.795 1.00 52.25
ATOM 1631 CE1 TVD 165	3 24.153 14.679 2.684 1.00.61.11
ATOM 1632 CD2 TYR 165	23.725 13.773 1.717 1 00 62 00
ATOM 1633 CE2 TVP 1CC	22.121 14.335 3 910 3 92.69
ATOM 1634 CZ TVB 165	21.685 13.429 2.953 1.00 66 22
ATOM 1635 OH TVD 1655	22.487 13.148 1 950 3
ATOM 1637 C TYR 1653	22.044 12.239 0.033
ATOM 1638 O TVR 165	23.733 16.313 7.345 1 00 63 40
ATOM 1639 N TVP 165	24.403 15.453 7 912 1 2
ATOM 1643	23.644 17.564 7 700
ATOM 1642 CD	24.379 18.013 8 963
ATOM 1643 00	24.947 19.417 8 741
ATOM 1644 cm	26.038 19.467 7.691 7.69
ATOM 1615	25.736 19.698 6.353 1.00 57.70
ATOM 1646 375	26.734 19.708 5 383 1.00 58.03
ATOM 1654	27.364 19.252 8.035 1.00 60.65
ATOM 1654	28.366 10.262 0.035 1.00 56.79
ATOM 1649 ON THE 1654	28.047 10 400
ATOM 1654	29.048 19.405 3.734 1.00 60.88
ATOM 1651 C TYR 1654	23.560 17 000 1.00 64.23
	23.560 17.980 10.239 1.00 65.89
SSCD/55115	

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PCT/US97/14885

MOTA	1652	0	TYR	1654	24.074	18.283	11.316	1.00	67.56
ATOM	1653	N	LYS	1655	22.297	17.586	10.135	1.00	67.36
ATOM	1655	CA	LYS	1655	21.443	17.527	11.315	1.00	69.11
ATOM	1656	CB	LYS	1655	19.972	17.611	10.915	1.00	69.86
MOTA	1657	CG	LYS	1655	19.019	17.651	12.090	1.00	71.45
MOTA	1658	CD	LYS	1655	17.607	17.867	11.603	1.00	75.40
ATOM	1659	CE	LYS	1655	16.595	17.393	12.627	1.00	78.22
ATOM	1660	NZ	LYS	1655	15.204	17.553	12.110	1.00	80.61
MOTA	1664	С	LYS	1655	21.714	16.242	12.093	1.00	69.65
MOTA	1665	0	LYS	1655	21.872	15.169	11.497	1.00	70.67
MOTA	1666	N	LYS	1656	21.766	16.358	13.419	1.00	68.19
ATOM	1668	CA	LYS	1656	22.035	15.212	14.275	1.00	68.00
MOTA	1669	C.B	LYS	1656	22.983	15.618	15.403	1.00	65.53
MOTA	1670	CG	LYS	1656	24.395	15.895	14.946	1.00	62.71
ATOM	1671	CD	LYS	1656	25.280	16.221	16.138	1.00	64.38
ATOM	1672	CE	LYS	1656	26.764	16.031	15.832	1.00	63.23
ATOM	1673	NZ	LYS	1656	27.592	16.186	17.062	1.00	61.72
ATOM	1677	C	LYS	1656	20.777	14.560	14.855	1.00	68.73
ATOM	1678	0	LYS	1656	19.695	15 148	14.837	1.00	69.20
MOTA	1679	N	THR	1657	20.928	13.337	15.359	1.00	68.48
ATOM	1681	CA	THR	1657	19.821	12.607	15.960	1.00	67.93
MOTA	1682	CB	THR	1657	20.109	11.078	16.021	1.00	68.93
MOTA	1683	OG1	THR	1657	21.295	10.823	16.787	1.00	68.72
MOTA	1685	CG2	THR	1657	20.289	10.50C	14.637	1.00	68.83
ATOM	1686	C	THR	1657	19.682	13.131	17.383	1.60	67.80
ATOM	1687	0	THR	1657	20.424	14.022	17.790	1.00	67.87
ATOM	1688	N	ALA	1658	18.753	12.569	18.148	1.00	68.95
MOTA	1690	CA	ALA	1658	18.580	12.992	19.537	1.00	70.64
ATOM	1691	CB	ALA	1658	17.391	12.254	20.173	1.00	71.19
ATOM	1692	С	ALA	1658	19.880	12.709	20.313	1.00	69.64
ATOM	1693	0	ALA	1658	20.394	13.566	21.042	1.00	70.13
ATOM	1694	Vi	ASN	1659	20.440	11.526	20.080	1.00	68.02
ATOM	1696	CA	ASN	1659	21.663	11.092	20.746		66.10
ATOM	1697	CB	ASN	1659	21.835	9.583	20.557		70.23
ATOM	1698	CG	ASN	1659	22.632	8.937	21.679		74.09
ATOM	1699	OD1		1659	22.525	9.331	22.840		75.21
ATOM	1700	ND2		1659	23.402	7.907	21.342		75.03
ATOM	1703	C	ASN	1659	22.910	11.816	20.249		63.30
ATOM	1704	0	ASN	1659		11.585	20.762		61.12
ATOM	1705	N	GLY	1660	22.744	12.678	19.246		61.61
MOTA	1707	CA	GLY	1660	23.867	13.421	18.689		59.06
ATOM	1708	С	GLY	1660	24.604	12.750	17.536		56.84
ATOM	1709	0	GLY	1660	25.726	13.132	17.196		55.69
ATOM	1710	N	ARG	1661	23.980	11.758	16.914		55.73
ATOM	1712	CA	ARG	1661	24.626	11.062	15.808		52.76
ATOM	1713	CB	ARG	1661	24.387	9.549	15.883		52.39
ATOM	1714	CG	ARG	1661	24.977	8.874	17.111	1.00	
ATOM	1715	CD	ARG	1661	24.776	7.376	17.045	1.00	
ATOM	1716	NE	ARG	1661	25.178	6.665	18.260	1.00	
ATOM	1718	CZ	ARG	1661	24.952	5.369	18.471	1.00	
ATOM	1719	NH1		1661	24.319	4.643	17.550	1.00	
ATOM	1722	NH2	AKG	1661	25.375	4.792	19.591	1.00	59.47



MOTA	1786	CE	MET	1667	21.033	9.447	2.341	1.00 38.17
ATOM	1787	C	MET	1667	24.042	4.960	3.276	1.00 25.07
ATOM	1788	0	MET	1667	25.256	5.037	3.411	1.00 27.61
MOTA	1789	N	ALA	1668	23.473	4.302	2.282	1.00 24.92
MOTA	1791	CA	ALA	1668	24.272	3.647	1.271	1.00 26.92
ATOM	1792	CB	ALA	1668	23.397	2.720	0.425	1.00 25.09
MOTA	1793	C	ALA	1668	24.866	4.759	0.410	1.00 27.82
MOTA	1794	0	ALA	1668	24.254	5.817	0.242	1.00 27.06
MOTA	1795	N	PRO	1669	26.050	4.530	-0.170	1.00 27.84
ATOM	1796	CD	PRO	1669	26.912	3.339	-0.107	1.00 27.12
ATOM	1797	CA	PRO	1669	26.662	5.561	-1.005	1.00 28.04
MOTA	1798	CB	PRO	1669	27.868	4.835	-1.593	1.00 26.71
ATOM	1799	CG	PRO	1669	28.249	3.893	-0.498	1.00 27.49
ATOM	1800	C	PRO	1669	25.734	6.078	-2.108	1.00 28.51
ATOM	1801	0	PRO	1669	25.685	7.281	-2.371	1.00 30.64
ATOM	1802	N	GLU	1670	24.992	5.179	-2.746	1.00 28.25
ATOM	1804	CA	GLU	1670	24.095	5.584	-3.826	1.00 26.82
MOTA	1805	CB	GLU	1670	23.600	4.369	4.620	1.00 29.32
ATOM	1806	CG	GLU	1670	22.604	3.486	-3.889	1.00 30.38
MOTA	1807	CD	GLU	1670	23.223	2.266	-3.229	1.00 32.52
ATOM	1808	OE1	GLU	1670	22.444	1.393	-2.794	1.00 28.06
MOTA	1809	OE2	GLU	1670	24.474	2.175	-3.130	1.00 28.67
MOTA	1810	C	GLU	1670	22.924	6.440	-3.356	1.00 24.79
ATOM	1811	0	GLU	1670	22.410	7.236	-4.123	1.00 22.31
MOTA	1812	N	ALA	1671	22.512	6.265	-2.101	1.00 26.70
ATOM	1814	CA	ALA	1671	21.423	7.040	-1.490	1.00 25.67
MOTA	1815	CB	ALA	1671	20.913	6.292	-0.312	1.00 18.88
MO1'A	1816	C	ALA	1671	21.984	8.365	-1.006	1.00 26.05
ATOM	1817	0	ALA	1671	21.400	9.414	-1.229	1.00 28.14
ATOM	1818	N	LEU	1672	23.138	8.300	-0.358	1.00 29.03
ATOM	1820	CA	LEU	1672	23.807	9.481	0.172	1.00 34.07
ATOM	1821	CB	LEU	1672	25.030	9.064	0.986	1.00 34.45
MOTA	1822	CG	LEU	1672	25.870	10.157	1.648	1.00 39.50
ATOM	1823		LEU	1672	25.081	10.853	2.740	1.00 41.71
MOTA	1824		LEU	1672	27.123	9.530	2.243	1.00 40.16
ATOM	1825	С	LEU	1672	24.248	10.431	-0.942	1.00 38.47
MOTA	1826	0	LEU	1672	23.958	11.625	-0.898	1.00 42.25
MOTA	1827	N	PHE	1673	24.924	9.901	-1.956	1.00 39.07
ATOM	1829	CA	PHE	1673	25.414	10.725	-3.053	1.00 38.00
ATOM	1830	CB	PHE	1673	26.699	10.110	-3.639	1.00 36.48
ATOM	1831	CG	PHE	1673	27.826	9.928	-2.637	1.00 33.36
ATOM	1832		PHE	1673	28.524	8.724	-2.580	1.00 29.55
ATOM	1833		PHE	1673	28.205	10.960	-1.779	1.00 31.85
ATOM	1834		PHE	1673	29.580	8.540	-1.692	1.00 26.33
ATOM	1835		PHE	1673	29.265	10.786	-0.880	1.00 30.95
MOTA	1836	CZ	PHE	1673	29.954	9.568	-0.838	1.00 28.99
ATOM	1837	С	PHE	1673	24.413	10.957	-4.194	1.00 39.64
ATOM	1838	0	PHE	1673	24.364	12.046	-4.760	1.00 37.72
ATOM	1839	N	ASP	1674	23.651	9.928	-4.554	1.00 41.35
ATOM	1841	CA	ASP	1674	22.716	10.027	-5.666	1.00 43.38
ATOM	1842	CB	ASP	1674	22.934	8.858	-6.625	1.00 47.84
ATOM	1843	CG	ASP	1674	24.359	8.765	-7.121	1.00 53.24

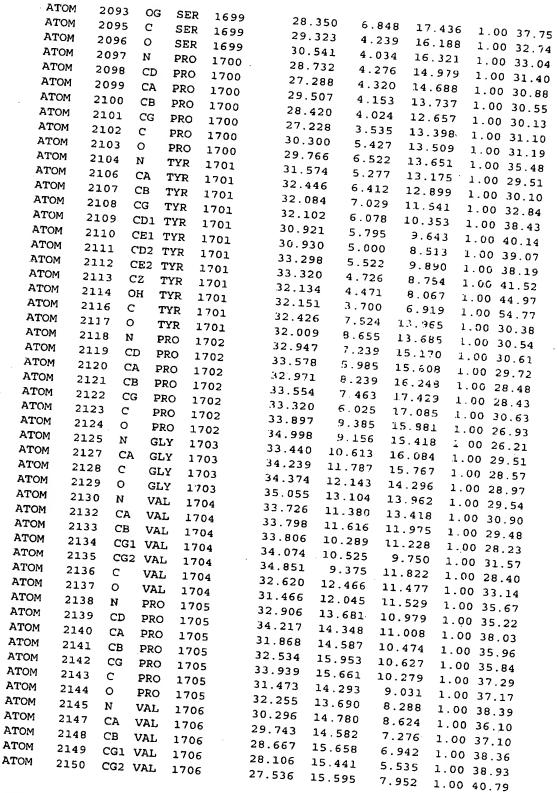
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	TOM 1845	OD2 AS	P 1674				.172 1	.00 56.20
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	OM 1847	O AS		21.		083 -5	.321 1	.00 45.94
	OM 1848	N AR		20.		200 -6.	222 1	.00 47.80
AT	OM 1850	CA ARC		20.				.00 45.98
AT		CB ARC	•	19.5				.00 43.76
ATO		CG ARC		18.8				.00 43.76
ATO		CD ARG		19.5		478 -3.		.00 58.37
ATC	DM 1854	NE ARG		19.4		715 -3.		00 38.37
ATC	DM 1856	CZ ARG		20.0	35 14.			00 70 39
ATC	M 1857	NH1 ARG		19.6	12 16.			00 79.14
ATO		NH2 ARG	_	18.6	10 16.3		_	00 82.95
ATO		_	1675	20.1	94 17.(			00 82.00
ATO		_	1675	18.6	47 8.8			00 87.42
ATO		O ARG	1675	17.46		· -		00 39.26
ATO		N ILE	1676	19.27		_		00 37.29
ATO		CA ILE	1676	18.54		-		00 35.86
ATON	4	CB ILE	1676	19.32		-		
ATOM	003	CG2 ILE	1676	18.45				00 31.73
ATOM		CG1 ILE	1676	19.76			-	00 30.02
		CD1 ILE	1676	20.65	_		19 1.0	00 32.68
ATOM		C ILE	1676	18.32			72 1.0	0 35.75
ATOM		O ILE	1676				16 1.0	0 31.08
ATOM		V TYR	1677	19.26			05 1.0	0 28.77
ATOM		'A TYR	1677	17.10	_		4 1.0	0 30.32
ATOM	-0,, (	B TYR	1677	16.779			8 T 00	0 29.68
ATOM		G TYR	1677	15.846		9 -1 35	- 1	0 31.14
ATOM		D1 TYR	1677	16.523		5 -0.51		32.95
ATOM		E1 TYR		16.616		1 -0.95		30.40
MOTA		70	1677	17.208		7 -0.17	-	27.57
ATOM		70	1677	17.048		2 0.74		7 47.57
ATOM	1883 C		1677	17.642	7.05			32.13
ATOM	1884 O		1677	17.711	8.366	1.08	_	
ATOM	1886 C		1677	18.235	9.326		_	
ATOM	1887 0		1677	16.123	3.424		1.00	32.18
ATOM	1888 N		1677	15.268	3.537		-	28.88
ATOM	200-	·	L678	16.556	2.253			32.20
ATOM			678	16.023	0.988			26.34
ATOM			.678	16.917	0.394		-	25.55
ATOM			678	18.221	0.179			28.81
ATOM			678	17.010	1.320			34.06
ATOM	1895 C		678	16.037	0.007	-5.267	_	27.25
ATOM	1896 O	THR 1	678	16.505	0.312		1.00	21.78
ATOM	1897 N	HIS 1	679	15.559	-1.198	-0.744	1.00	25.57
	1899 CA	HIS 1	679	15.580		-2.071	1.00	20.86
ATOM	1900 CB		579	14.816	-2.216	-1.030	1.00	20.30
ATOM	1901 CG	HIS 16	579	13.367	-3.453	-1.499	1.00	17.22
ATOM	1902 CD2		579		-3.196	-1.797	1.00	19.02
ATOM			79	12.662	-3.275	-2.958	1.00	14.89
ATOM			79	12.459	-2.830	-0.826	1.00 ]	18.98
ATOM			79	11.260	-2.697	-1.370	1.00 1	16 10
ATOM	1908 C		79	11.359	-2.961	-2.663	1.00 1	5 10
ATOM	1909 O		79 79	17.050	-2.535	-0.761	1.00 2	0.10
	_	TP	13	17.428	-2.901	0.356	1.00 2	2 50
							2.00 2	4.38

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ATOM	1910	N	GLN	1680	17.874	-2.310	-1.781	1.00 20.58
ATOM	1912	CA	GLN	1680	19.303	-2.539	-1.721	1.00 22.70
ATOM	1913	CB	GLN	1680	19.935	-2.427	-3.106	1.00 26.26
ATOM	1914	CG	GLN	1680	19.934	-3.711	-3.889	1.00 31.86
ATOM	1915	CD	GLN	1680	18.949	-3.687	-5.026	1.00 37.54
ATOM	1916	OE1	GLN	1680	17.931	-3.000	-4.961	1.00 42.70
ATOM	1917	NE2	GLN	1680	19.256	-4.409	-6.091	1.00 37.42
ATOM	1920	С	GLN	1680	19.985	-1.559	-0.797	1.00 24.93
ATOM	1921	0	GLN	1680	20.875	-1.943	-0.039	1.00 26.39
MOTA	1922	N	SER	1681	19.605	-0.286	-0.867	1.00 24.70
ATOM	1924	CA	SER	1681	20.239	0.678	0.030	1.00 23.24
ATOM	1925	CB	SER	1681	19.923	2.128	-0.346	1.00 19.33
ATOM	1926	OG	SER	1681	18.544	2.326	-0.545	1.00 18.55
ATOM	1928	C	SER	1681	19.852	0.364	1.464	1.00 21.77
ATOM	1929	0	SER	1681	20.645	0.609	2.366	1.00 24.14
ATOM	1930	N	ASP	1682	18.659	-0.210	1.670	1.00 21.80
MOTA	1932	CA	ASP	1682	18.180	-0.604	3.003	1.00 22.45
MOTA	1933	CB	ASP	1682	16.730	-1.111	2.963	1.00 25.27
MOTA	1934	CG	ASP	1682	15.678	0.004	3.132	1.00 28.21
MOTA	1935	OD1	ASP	1682	14.500	0.245	2.786	1.00 25.41
MOTA	1936	OD2	ASP	1682	15.992	1.102	3.639	1.00 30.19
ATOM	1937	C	ASP	1682	19.076	-1.736	3.517	1.00 23.69
ATOM	1.938	O	ASP	1682	19.385	-1.799	4.709	1.00 24.74
ATOM	1939	11	VAL	1683	19.474	-2.635	2.620	1.00 23.49
ATOM	1941	CA	VAL	1683	20.354	-3.737	3.003	1.00 21.77
ATOM	1942	CB	VAL	1683	20.543	-4.741	1.837	1.00 20.49
MOTA	1943	CG1	VAL	1683	21.770	5.613	2.039	1 00 19.82
MOTA	1944	CG2	VAL	1683	19.320	-5.618	1.736	1.00 19.29
MOTA	1945	C	.IAV	1683	21.674	-3.153	3.523	1.00 21.93
ATOM	1946	O	VAL	1683	22.161	-3.570	4.573	1.00 21.06
ATOM	1947	N	TRP	1684	22.207	-2.143	2.837	1.00 20.64
ATOM	1949	CA	TRP	1684	23.424	-1.482	3.295	1.00 20.98
ATOM	1950	CB	TRP	1684	23.711	-0.224	2.463	1.00 19.56
ATOM	1951	CG	TRP	1684	24.859	0.609	2.970	1.00 23.22
ATOM	1952	CD2	TRP	1684	26.182	0.686	2.421	1.00 24.64
ATOM	1953	CE2	TRP	1684	26.929	1.559	3.249	1.00 24.69
MOTA	1954	CE3	TRP	1684	26.813	0.102	1.315	1.00 26.41
A'TOM	1955	CD1	TRP	1684	24.857	1.430	4.075	1.00 23.64
ATOM	1956	NE1	TRP	1684	26.097	1.994	4.246	1.00 23.28
ATOM	1958	CZ2	TRP	1684	28.275	1.859	3.000	1.00 20.55
MOTA	1959	CZ3	TRP	1684	28.165	0.409	1.072	1.00 22.82
ATOM	1960	CH2	TRP	1684	28.872	1.274	1.908	1.00 19.24
ATOM	1961	C	TRP	1684	23.201	-1.112	4.771	1.00 21.12
ATOM	1962	0	TRP	1684	23.931	-1.560	5.652	1.00 22.08
MOTA	1963	N	SER	1685	22.150	-0.342	5.032	1.00 23.27
ATOM	1965	CA	SER	1685	21.787	0.086	6.386	1.00 22.54
MOTA	1966	CB	SER	1685	20.429	0.768	6.356	1.00 21.98
MOTA	1967	OG	SER	1685	20.318	1.626	5.220	1.00 25.48
ATOM	1969	С	SER	1685	21.747	-1.068	7.389	1.00 21.33
ATOM	1970	0	SER	1685	22.145	-0.902	8.545	1.00 19.52
MOTA	1971	N	PHE	1686	21.260	-2.228	6.946	1.00 23.10
ATOM	1973	CA	PHE	1686	21.174	-3.424	7.800	1.00 23.09

ATO		CB p	HE 1686	20.4				
ATO	, -		HE 1686	20.4		550 7.	095 1.00 22.7	7
ATC		CD1 P		20.1 19.3			962 1.00 25.8	2
ATC		CD2 P		20.8	-		096 1.00 25.54	
ATO		CE1 P	HE 1686	19.1			649 1.00 23.88	8
ATO	-5,5	CE2 P	HE 1686	20.62			913 1.00 24.25	5
ATO		CZ P	HE 1686	19.80			155 1.00 22.67	7
ATO		C PI	HE 1686	22.56			85 1.00 26.30	)
ATO	-502	O PI		22.73		_	,	
ATO		N GI		23.55				,
ATON	_	CA GI	Y 1687	24.91				
ATOM	_	C GL	Y 1687	25.40			85 1.00 19.29	
ATOM		O GL	Y 1687	26.09	_			
ATOM		N VA		25.00			15.40	
ATOM		CA VA		25.37				
ATOM		CB VA	L 1688	25.04				
ATOM		CG1 VA	1688	25.43			20.20	
ATOM		CG2 VA	1688	25.820				
ATOM		C VAI		24.621				
ATOM ATOM	1995	IAV O	1688	25.204				
ATOM		N LEU	J 1689	23.339				
ATOM		CA LEU	- 305	22.542				
ATOM		CB LEU		21.072			2.	
ATOM		CG TEA		19.981			* ~~, , , ,	
ATOM		CD1 LEU		18.614				
ATCM		CD2 LEU	_	20.048				
ATOM		LEU	1689	23.158			, ,	
ATOM			1689	23.202	-3.592			
ATOM	500		1690	23.514	-4.379	11.87		
ATOM		A LEU B LEU	1690	24.256	-5.604			
ATOM			1690	24.730	-6.531			
ATOM	_	G LEU	1690	23.809	-7.501			
ATOM		D2 LEU	1690	24.662	-8.259	9.523		
ATOM	2012 C		1690	23.135	-8.487	11.458		
ATOM	2013 0	LEU	1690	25.471	-5.204	13.189		
ATOM	2014 N	TRP	1690	25.710	-5.747	14.273	1.00 29.07	
ATOM	2016 C		1691 1691	26.240	-4.255	12.660	1.00 26.26	
ATOM	2017 CE		1691	27.431	-3.761	13.341	1.00 25.08	
ATOM	2018 CC		1691	28.129	-2.706	12.493	1.00 25.16	
ATOM	2019 CI	2 TRP	1691	29.456	-2.268	13.039	1.00 27.49	
ATOM		2 TRP	1691	29.701	-1.163	13.925	1.00 25.81	
ATOM		3 TRP	1691	31.100	-1.070	14.103	1.00 22.63	
ATOM		1 TRP	1691	28.870	-0.236	14.575	1.00 26.70	
ATOM		1 TRP	1691	30.688	-2.798	12.735	1.00 23.03	
ATOM		2 TRP	1691	31.675	-2.078	13.371	1.00 25.19	
ATOM			1691	31.690	-0.085	14.900	1.00 18.66	
ATOM	2027 CH		1691	29.459	0.745	15.371	1.00 25.66	
ATOM	2028 C		1691	30.861	0.812	15.523	1.00 23.00	
	2029 O		1691		-3.195	14.727	1.00 24.63	
	2030 N		1692	_	-3.393	15.662	1.00 27.79	
MOTA	2032 CA		1692		-2.506	14.862	1.00 26.48	
			-	23.3/4 .	-1.938	16.155	1.00 24.98	

**ATOM** 2033 CB GLU 1692 15.994 24.335 -1.060 1.00 22.29 ATOM 2034 CG GLU 1692 24.507 0.107 15.056 1.00 18.31 ATOM 2035 CD GLU 1692 23.255 0.933 14.978 1.00 25.10 2036 **ATOM** OE1 GLU 1692 22 433 0.704 14.066 1.00 26.95 **ATOM** 2037 OE2 GLU 23.067 1692 1.815 15.840 1.00 27.05 ATOM 2038 С GLU 1692 25.260 -3.036 17.163 1.00 25.18 ATOM 2039 0 GLU 1692 25.602 -2.927 18.341 1.00 26.12 ATOM 2040 N ILE 1693 24.593 -4.087 16.698 1.00 27.16 **ATOM** 2042 CA ILE 1693 24.231 -5.214 17.555 1.00 25.91 **ATOM** 2043 CB ILE 1693 23.373 -6.287 16.777 1.00 25.70 -7.564 ATOM 2044 CG2 ILE 1693 23.171 17.638 1.00 18.73 ATOM 2045 CG1 ILE 1693 22.005 -5.682 16.382 1.00 23.45 ATOM 2046 CD1 ILE 1693 21.208 -6.485 15.346 1.00 15.62 ATOM 2047 ILE 1693 C 25.496 -5.847 18.107 1.00 26.70 ATOM 2048 0 ILE 1693 25.672 -5.961 19.316 1.00 28.19 MOTA 2049 PHE N 1694 26.442 -6.133 17.229 1.00 28.78 MOTA 2051 CA PHE 1694 27.664 -6.779 17.679 1.00 29.72 **ATOM** 2052 CB PHE 1694 28.261 -7.598 16.542 1.00 27.18 MOTA 2053 CG PHE 1694 27.315 -8.649 16.048 1.00 25.38 **ATOM** 2054 CD1 PHE 1694 26.793 -8.599 14.770 1.00 26.16 ATOM CD2 PHE 2055 1694 . 26.844 -9.625 16.919 1.00 26.37 ATOM 2056 CE1 PHE 1694. 25.808 -9.505 14.370 1.00 31.37 ATOM 2057 CE2 PHE 1694 25.863 -10.533 16.536 1.00 25.23 MOTA 2058 CZPHE 15.268 . 1694 25.337 -10.478 1.00 29.46 **ATOM** 2059 C PHE 1694 28.663 -5.906 18.438 1.00 30.92 ATOM PHE 2060 0 1694 29.697 -6.403 18.902 1.00 32.23 **ATOM** 5061 N THR 1695 28.344 -4.616 18.575 1.00 29 46 **ATOM** 2063 CA THR 1695 29.170 -3.698 19.348 1.00 27.17 ATOM 2064 CB THR 1695 29.665 -2.474 18.535 1.00 23.32 ATOM OG1 THR 2065 1695 28.553 -1.710 18.046 1.00 24.73 ATOM 2067 CG2 THR 1695 30.538 -2.914 17.395 1.00 21.34 MOTA 2068 С THR 1695 28.307 -3.230 20.519 1.00 28.81 ATOM 2069 O THR 1695 28.707 -2.346 21,289 1.00 31.85 ATOM 2070 N LEU 1696 27.130 -3.841 20.651 1.00 26.30 **ATOM** 2072 CA LEU 1696 26.188 -3.523 21.720 1.00 25.99 MOTA 2073 CB LEU 1696 26.704 -4.043 23.060 1.00 24.51 MOTA 2074 CG LEU 1696 26.974 -5.539 23.194 1.00 23.32 MOTA 2075 CD1 LEU -5.843 1696 27.447 24.597 1.00 26.45 **ATOM** 2076 CD2 LEU 1696 25.726 -6.297 22.907 1.00 29.79 ATOM 2077 С LEU 1696 25.892 -2.036 21.837 1.00 24.90 ATOM 2078 0 LEU 1696 26.083 -1.457 22.889 1.00 28.99 **ATOM** 2079 GLY N 1697 25.386 -1.43220.771 1.00 25.05 MOTA 2081 CA GLY 1697 25.072 -0.016 1.00 24.31 20.811 MOTA 2082 C GLY 1697 26.241 0.847 20.381 1.00 27.15 MOTA 2083 0 GLY 1697 26.297 2.035 20.701 1.00 29.57 MOTA 2084 N GLY 1698 27.177 0.261 19.639 1.00 27.33 **ATOM** 2086 CA GLY 1698 28.319 1.023 19.178 1.00 27.04 **ATOM** 2087 C GLY 1698 27.966 2.109 18.173 1.00 29.78 MOTA 2088 GLY 17.301 0 1698 27.115 1.929 1.00 32.03 MOTA 2089 SER N 1699 28.633 3.247 18.295 1.00 30.60 ATOM 2091 CA SER 1699 28.413 4.385 17.414 1.00 31.48 ATOM 2092 CB SER 1699 28.747 5.692 18.164 1.00 32.97



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ATOM	2151	C	VAL	1706	30.762	14.559	6.138	1.00	37.09
ATOM	2152	0	VAL	1706	30.927	13.543	5.461	1.00	38.75
ATOM	2153	N	GLU	1707	31.477	15.663	5.967	1.00	37.08
ATOM	2155	CA	GLU	1707	32.472	15.793	4.910	1.00	35.52
MOTA	2156	CB	GLU	1707	33.059	17.206	4.918	1.00	38.30
ATOM	2157	С	GLU	1707	33.588	14.762	4.945	1.00	34.20
ATOM	2158	0	GLU	1707	34.153	14.445	3.908	1.00	33.48
MOTA	2159	N	GLU	1708	33.936	14.273	6.132	1.00	34.20
MOTA.	2161	ÇA	GLU	1708	34.981	13.256	6.241	1.00	36.08
MOTA	2162	CB	GLU	1708	35.555	13.178	7.660	1.00	40.39
MOTA	2163	CG	GLU	1708	36.212	14.464	8.179	1.00	45.41
MOTA	2164	CD	GLU	1708	37.471	14.871	7.430	1.00	50.66
ATOM	2165	OE1	GLU	1708	38.199	13.986	6.909	1.00	54.73
ATOM	2166	OE2	GLU	1708	37.747	16.092	7.392	1.00	52.85
MOTA	2167	C	GLU	1708	34.369	11.911	5.855	1.00	35.22
ATOM	2168	0	GLU	1708	35.035	11.045	5.260	1.00	34.04
ATOM	2169	N	LEU	1709	33.089	11.745	6.178	1.00	33.30
MOTA	2171	CA	LEU	1709	32.376	10.519	5.860		31.44
ATOM	2172	CB	LEU	1709	30.975	10.531	6.474	1.00	26.89
MOTA	2173	CG	LEU	1709	30.065	9.366	6.073	1.00	26.05
MOTA	2174	CD1	LEU	1709	30.652	8.036	6.503	1.00	22.75
ATOM	2175	CD2	LEU	1709	28.717	9.574	6.597	1.00	26.15
ATOM	2176	C	LEU	1709	32.291	10.325	4.350	1.00	31.18
ATOM	2177	0	LEU	1709	32.490	9.209	3.858	1.00	29.88
ATOM	2178	N	PHE	1710	32.011	11.408	3.623	1.00	30.16
ATOM	2180	CA	PHE	1710	31.915	11.333	2.169		31.64
ATOM	2181	CB	PHE	1710	31.658	12.710	1.567		33.44
ATOM	2182	CG	PHE	1710	30.287	13.231	1.827	1.00	37.78
ATOM	2183		PHE	1710	29.287	12.395	2.303		41.46
ATOM	2184	CD2	PHE	1710	29.991	14.565	1.613	1.00	40.72
ATOM	2185	CE1	PHE	1710	28.012	12.882	2.566		41.30
ATOM	2186		PHE	1710	28.715	15.058	1.875		42.99
ATOM	2187	CZ	PHE	1710	27.725	14.208	2.354	1.00	4C.95
ATOM	2188	Ç	PHE	1710	33.202	10.771	1.609		32.38
ATOM	2189	0	PHE	1710	33.183	9.815	0.825		32.26
ATOM	2190	N	LYS	1711	34.310	11.336	2.085		31.26
MOTA	2192	CA	LYS	1711	35.664	10.971	1.697		29.73
MOTA	2193	CB	LYS	1711	36.642	11.932	2.379		33.49
ATOM	2194	CG	LYS	1711	38.103	11.716	2.042		39.79
ATOM	2195	CD	LYS	1711	38.981	12.731	2.755		43.35
ATOM	2196	CE	LYS	1711	40.413	12.686	2.238		<b>4€.23</b>
ATOM	2197	NZ	LYS	1711	41.116	11.422	2.600		53.67
ATOM	2201	C	LYS	1711	35.999	9.501	2.015		29.34
ATOM	2202	0	LYS	1711	36.670	8.836	1.231		28.77
ATOM	2203	И	LEU	1712	35.541	9.000	3.164		30.40
ATOM	2205	CA	LEU	1712	35.776	7.599	3.532	1.00	
ATOM	2206	CB	LEU	1712	35.241	7.295	4.942	1.00	
ATOM	2207	CG	LEU	1712	35.971	7.870	6.166	1.00	
ATOM	2208	CD1		1712		7.593	7.440	1.00	
ATOM	2209	CD2		1712	37.389	7.297	6.266	1.00	
ATOM	2210	С	LEU	1712	35.022	6.738	2.530	1.00	
ATOM	2211	0	LEU	1712	35.571	5.796	1.957	1.00	29.28

ATO		N LEU	1713	2.2				
ATON		CA LEU	1713			.073 2	.325 1.00 31.9	Ω
ATOM		CB LEU	1713			.339 1	.403 1.00 34.3	in.
ATOM		CG LEU	1713				·447 1.00 37.6	5
ATOM	,	CD1 LEU	1713			450 2	.686 1.00 37.0	5
ATOM	0	CD2 LEU	1713			217 2	781 1.00 36 8	0
ATOM		C LEU	1713		4		641 1.00 37.0	2
ATOM		_	1713	33.		344 -0.	011 1.00 35.49	5
ATOM			1714	33.4			662 1.00 38.78	3
ATOM	2223		1714	33.9			<sup>481</sup> 1.00 33.22	
ATOM	2224	(ID)	1714	34.4 34.8		590 -1.	821 1.00 31 46	
ATOM	2225	00	1714	33.7		027 -2.	158 1.00 31 35	
ATOM ATOM	2226	CD LYS 1	1714	32.8			<sup>399</sup> 1.00 33 <sub>.49</sub>	
	2227	CC 7114	714	31.6			<sup>191</sup> 1.00 39.40	
ATOM	2228	NZ LYS 1	714	30.6	_		720 1.00 44.79	
ATOM ATOM	2232	C LYS 1	714	35.7			71 1.00 50.41	
	2233	^	714	35.9	_		153 1.00 32.53	
ATOM ATOM		N GLU 1	715	36.42		· <del>-</del>	25 1.00 35.46	
ATOM			715	37.60			56 1.00 33.50	
ATOM	200-		715	38.61			64 1.00 34 92	
ATOM	20	$\mathtt{CG}$ $\mathtt{GLU}$ $\mathtt{1}.$	715	39.08			43 1.00 37.20	
ATOM	00	CD GLU 1	715	39.65			21 1.00 44.59	
ATOM			715	39.82		_		
ATOM		DE2 GLU 17	15	39.93		_		
ATOM	2242	020 17	15	37.27				
ATOM	2243 C	420 1,	15	38.18	4 3,35			
ATOM				35.99	1 3.86	-		
ATOM		A GLY 17		35.576	5 2.49	_		
ATOM	2247 C			35.852				
ATOM	2249 N	17.		35.906			-2.00	
ATOM	2251 C	1.7.		35.995	2.879			
	2252 CI			36.282	2.489		0.10	
	2253 CC	1/1		36.534	3.743		+ ->.00	
ATOM		10		36.794	3.469			
ATOM		17 79		37.955	3.375			
				35.782	3.279			
ATOM 2		2		36.309	3.080	7.942		
	2260 c	HIS 171		37.624	3.134	7.830		
ATOM 2	2261 0	HIS 171		35.171	1.645	4.153		
ATOM 2	262 N	ARG 1718		33.987	1.900	3.940	1.00 31.43	
	264 CA	ARG 1718		35.571	0.666	4.955	1.00 28.11	
ATOM 2	265 CB	ARG 1718		34.632	-0.212	5.640	1.00 30.67	
	266 CG	ARG 1718		34.592	-1.583	4.973	1.00 27.32	
ATOM 2	267 CD	ARG 1718		34.058	~1.586	3.557	1.00 28.77	
ATOM 2	268 NE	ARG 1718		32.609	-1.111	3.484	1.00 28.84	
	270 CZ	ARG 1718		32.032	-1.167	2.131	1.00 24.96	
	271 NH1	ARG 1718		32.141	-0.206	1.204	1.00 23.90	
	274 NH2	ARG 1718		32.824	0.912	1.454	1.00 20.04	
	277 C	ARG 1718		31.513	-0.338	0.045	1.00 20.04	
	278 O	ARG 1718		35.091	-0.350	7.101	1.00 33.92	
ATOM 22	279 N	MET 1719		36.300	-0.449	7.377	1.00 36.48	
				34.134	-0.355	8.028	1.00 33.22	



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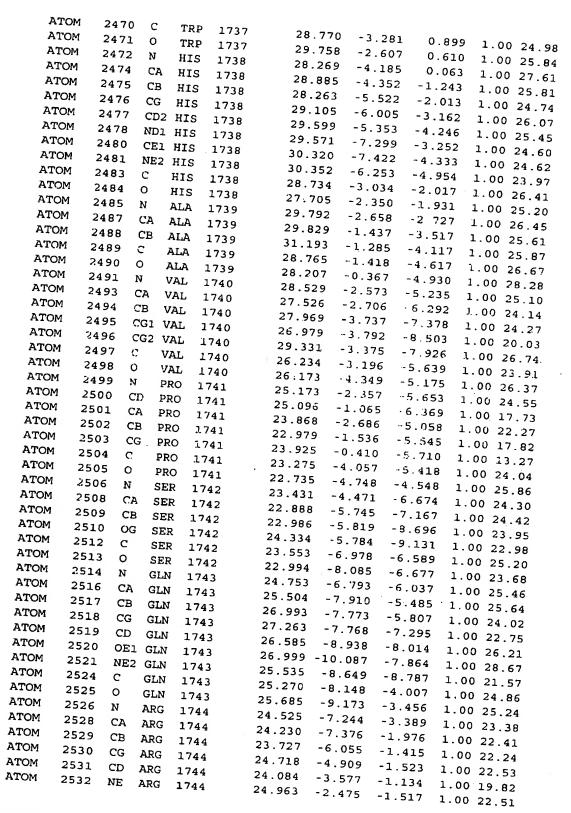
ATOM	2281	CA	MET	1719	34.428		9.448	1.00 32.33
ATOM	2282	CB	MET	1719	33.148		10.277	1.00 34.72
MOTA	2283	CG	MET	1719	32.454		10.076	1.00 35.04
MOTA	2284	SD	MET	1719	31.025		11.141	1.00 34.06
MOTA	2285	CE	MET	1719	29.757		10.409	1.00 33.14
ATOM	2286	С	MET	1719	35.068	-1.797	9.747	1.00 35.53
ATOM.	2287	0	MET	1719	34.896	-2.756	8.991	1.00 35.48
ATOM	2288	N	ASP	1720	35.826	-1.843	10.840	1.00 38.65
ATOM	2290	CA	ASP	1720	36.521	-3.049	11.281	1.00 39.03
ATOM	2291	CB	ASP	1720	37.659	-2.678	12.237	1.00 43.11
ATOM	2292	CG	ASP	1720	38.743	-1.846	11.569	1.00 46.69
ATOM	2293	OD1	ASP	1720	38.587	-1.536	10.364	1.00 54.08
ATOM	2294	OD2	ASP	1720	39.750	-1.503	12.239	1.00 45.93
ATOM	2295	C	ASP	1720	35.580	-4.023	11.972	1.00 38.50
MOTA	2296	0	ASP	1720	34.554	-3.617	12.528	1.00 37.73
MOTA	2297	N	LYS	1721	35.961	··5.298	11.981	1.00 38.10
MOTA	2299	CA	LYS	1721	35.151	-6.339	12.600	1.00 38.12
ATOM	2300	CB	LYS	1721	35.727	-7.733	12.323	1.00 38.20
MOTA	2301	CG	LYS	1721	34.825	-8.858	12.825	1 00 38.48
ATOM	2302	CD	LYS	1721	35.375	-19.238	12.543	1.00 37.49
MOTA	2303	CE	LYS	1721	36.320	-3.0.691	13.625	1.00 39 11
MOTA	2304	NZ	LYS	1721	36.448	-12.167	13.628	1.00 40.75
MOTA	2308	C	LYS	1721	35.092	-6.142	14.091	1.00 40.24
ATOM	2309	0	LYS	1721	. 36.136	-6.032	14 739	1.00 42.70
MOTA	2310	N	PRO	1722	33.875	-6.082	14.658	1.00 41.23
MOTA	2311	ÇD	PRO	1722	32.547	-6.153	14.019	1.00 38.63
MOTA	2312	CA	PRO	1722	33.743	-5.901	16.104	1.00 41.71
A'TOM	2313	CB	PRO	1722	32.223	-5.957	16.306	1.00 38.90
ATOM	2314	CG	PRO	1722	31.679	-5.442	15.016	1.00 34.19
ATOM	2315	C	PRO	1722	34.418	-7.079	16.819	1.00 43.96
MOTA	2316	O	PRO	1722	34.542	-8.174	16.250	1.00 43.02
ATOM	2317	N	SER	1723	34.915	-6.860	18.028	1.00 46.76
MOTA	2319	CA	SER	1723	35.493	-7.973	18.747	1.00 50.74
MOTA	2320	CB	SER	1723	36.265	-7.500	19.980	1.00 49.47
MOTA	2321	OG	SER	1723	35.400	-7.130	21.035	1.00 53.87
MOTA	2323	C	SER	1723	34.259	-8.782	19.143	1.00 53.24
ATOM	2324	0	SER	1723	33.136	-8.259	19.130	1.00 53.97
ATOM	2325	N	ASN	1724	34.443	-10.064	19.426	1.00 56.59
MOTA	2327	CA	ASN	1724	33.316	-10.899	19.825	1.00 59.55
ATOM	2328	CB	ASN	1724	32.739	-10.386	21.162	1.00 66.12
ATOM	2329	CG	ASN	1724	33.824	-10.128	22.213	1.00 71.34
ATOM	2330	OD1	ASN	1724	34.661	-10.990	22.485	1.00 73.38
ATOM	2331	ND2	ASN	1724	33.831	-8.926	22.779	1.00 74.19
ATOM	2334	C	ASN	1724	32.256	-10.900	18.711	1.00 57.31
ATOM	2335	0	ASN	1724	31.073	-10.662	18.940	1.00 59.27
ATOM	2336	N	CYS	1725	32.723	-11.132	17.493	1.00 54.50
ATOM	2338	CA	CYS	1725		-11.203	16.300	1.00 50.89
ATOM	2339	CB	CYS	1725	31.827	-9.848	15.576	1.00 50.09
ATOM	2340	SG	CYS	1725	30.893	-9.833	14.006	1.00 44.81
MOTA	2341	С	CYS	1725		-12.235	15.439	1.00 47.28
ATOM	2342	0	CYS	1725		-12.172	15.288	1.00 48.97
ATOM	2343	N	THR	1726	31.863	-13.229	14.950	1.00 42.60

_					
		2345		THR 172	6
		2346		THR 172	32.3/2 -14.275 14 120 7 22
	TOM	2347	OG1	- · - ·	31.520 -15,494 13 994 1 3
	TOM :	2349	CG2		30.290 -15.087 13 362 3 3
		2350	С	THR 1726	31.210 -16.084 15 326 1 20
	rom 2	2351	0		32.858 -13.748 12 776 1 22
	COM 2	2352	N		32.373 -12.704 12.357
	OM 2	354	CA	,	33.724 -14.473 12 080 7 1.00 39.57
AT	OM 2	355	CB		34.133 -14.044 10 742 7
	'OM 2	356	CG		35.290 -14.880 10 221
AT		357	OD1		36.580 -14.593 10.953 1.55
ATO		358	ND2		37.188 -13.539 10 781 1 79
ATO	~	361			37.010 -15 536 1.00 46.57
ATO	~	362	_	ASN 1727	32.958 -14 150 - 1.00 48.30
ATO		363		ASN 1727	32.883 -12 423
ATC		65	`	GLU 1728	32.041 -15 026
ATO		66		3LU 1728	30.854 -15 373
ATO		67		LU 1728	30.109 -16 553
ATO.			_	LU 1728	28.973 -17 000 2 7.765 1.00 32.82
ATO				LU 1728	28.329 -18 306 - 1.00 35.84
ATO			OE1 G		28.409 18 633
ATO		_	OE2 G	_	27.734 -18.005
ATON				LU 1728	29 925 1. 936 8.440 1.00 38.81
ATOM				LU 1728	29 521 9.313 1.00 33.05
ATOM				EU 1729	29 600 15 8.272 1.00 29.58
ATOM				EU 1729	28 743 15 10.527 1.00 32 09
ATOM			B LE	U 1729	28 351 12.330 10.710 1.00 32.46
ATOM		-	G LE		27 311 -2.309 12.170 1.00 32.64
ATOM			D1 LE	U 1729	27 121 23.431 12.575 1.00 34.65
ATOM	,		D3 FE	U 1729	25 990 14.089 1.00 37.18
			LE		29 350 11.842 1.00 27 77
ATOM		**	LE		44.434 (0) 175 1 00
ATOM	2382		TY	R 1730	30 600 9.693 1.00 31 97
ATOM	2384		A TY		10.251 1 00 31 70
ATOM	2385		TYP		32 040 9.734 1.00 30 19
ATOM	2386		TYF		32.849 -9.940 10.154 1 00 27 25
ATOM	2387		1 TYR		33.591 -8.723 9.649 1.00 35 53
ATOM	2388		1 TYR		33.093 -7.449 9.879 1.00 27 25
ATOM	2389		2 TYR		33.725 -6.324 9.378 1 00 37 56
ATOM	2390	CE	2 TYR	1730	34.759 -8.849 8.904 1.00 24.07
MOTA	2391	CZ			33.408 -7.724 8.393 1.00 24.01
ATOM	2392	ОН	TYR		34.882 -6.462 8.631 1.00 20
ATOM	2394	С	TYR	1730	35.4/3 -5.316 8.111 1.00 20.50
ATOM	2395	0	TYR	1730	31.287 -9.962 8.208 1.00 29.08
ATOM	2396	N	MET		31.062 -8.928 7 585 1 22
ATOM	2398	CA	MET	1731	31.443 -11.139 7 623 13 25
ATOM	2399	СВ	MET	1731	31.366 -11.313 6 187 1 00 31.05
ATOM	2400	CG	MET	1731	31.611 -12.779 5 840 1 00
ATOM	2401	SD		1731	31.315 -13.149 4 403 1 22
ATOM	2402	CE	MET	1731	31.801 -14.840 3 994
ATOM	2403	CE	MET	1731	32.926 -14.502 2 606 3 64.38
ATOM	2404		MET	1731	29 992 10 252
ATOM	2405	N	MET	1731	29.863 -10.36
		14	MET	1732	28 971 _11 152
					28.971 -11.153 6.501 1.00 33.32
SSSD/cc.					

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MOTA	2407	CA	MET	1732	27.594	-10.770	6.194	1.00 31.78
ATOM	2408	CB	MET	1732	26.634	-11.346	7.236	1.00 30.42
MOTA	2409	CG	MET	1732	25.172	-11.071	6.938	1.00 30.28
ATOM	2410	SD	MET	1732	24.071	-11.709	8.183	1.00 27.41
MOTA	2411	CE	MET	1732	23.738	-13.369	7.471	1.00 22.35
MOTA	2412	Ç	MET	1732	27.484	-9.243	6.158	1.00 31.10
ATOM	2413	0	MET	1732	26.794	-8.680	5.303	1.00 31.08
MOTA	2414	N	MET	1733	28.139	-8.586	7.114	1.00 31.22
MOTA	2416	CA	MET	1733	28.161	-7.128	7.189	1.00 30.93
MOTA	2417	CB	MET	1733	29.001	-6.665	8.376	1.00 31.91
ATOM	2418	CG	MET	1733	28.368	-6.906	9.710	1.00 33.63
ATOM	2419	SD	MET	1733	29.375	-6.210	11.021	1.00 34.53
ATOM	2420	CE	MET	1733	29.106	-7.395	12.280	1.00 34.12
ATOM	2421	C	MET	1733	28.830	-6.623	5.921	1.00 32.49
MOTA	2422	0	MET	1733	28.357	-5.682	5.281	1.00 33.61
ATOM	2423	N	ARG	1734	29.932	-7.269	5.551	1.00 32.11
ATOM	2425	CA	ARG	1734	30.673	-6.889	4.355	1.00 31.13
MOTA	2426	CB	ARG	1734	32.012	-7.623	4.308	1.00 28.68
ATOM	2427	CG	ARG	1734	32.953	-7.267	5.451	1. 00 27.19
ATOM	2428	CD	ARG	1734	33.159	-5.766	5.558	1.00 26.80
ATOM	2429	NE	ARG	1734	33.864	-5.243	4.393	1.00 35.67
ATOM	2431	CZ	ARG	1734	35.187	-5.305	4.223	1.00 38.03
ATOM	2432		ARG	1734	35.967	-5.861	5.148	1 00 38.07
ATOM	2435		ARG	1734	35.729	-4.850	3.094	1.00 38.87
ATOM	2438	C	ARG	1734	29.873	-7.098	3.065	1.00 29.53
MOTA	2439	O	ARG	1734	30.029	-6.334	2.121	1.00 29.11
ATOM	2440	N	ASP	1735	29.036	-8.137	3.025	1.00 29.48
ATOM	2442	CA	ASP	1735	28.193	-8.412	1.859	1.00 26.82
ATOM	2443	CB	ASP	1735	27.591	-9.811	1.933	1.00 30.25
ATOM	2444	CG	ASP	1735	28.632	-10.895	1.773	1.00 35.13
ATOM	2445	ODI		1735		-10.645	1.052	1.00 35.19
ATOM	2446	OD2		1735		-11.990	2.366	1.00 39.35
MOTA	2447	C	ASP	1.735	27.082	-7.375	1.760	100 23.88
ATOM	2448	0	ASP	1735		-6.992	0.656	1.00 24.83
MOTA	2449	И	CYS	1736	26.574	-6.929	2.913	1.00 22.13
ATOM	2451	CA	CYS	1736	25.538	-5.887	2.965	1.00 21.74
ATOM	2452	CB	CYS	1736	25.005	-5.692	4.401	1.00 20.46
ATOM	2453	SG	CYS	1736	23.978	-7.013	5.053	1.00 19.59
ATOM	2454	С	CYS	1736	26.104	-4.542	2.456	1.00 20.51
ATOM	2455	0	CYS	1736	25.377	-3.732	1.887	1.00 16.07
ATOM	2456	N	TRP	1737	27.401	-4.325	2.670	1.00 21.58
MOTA	2458	CA	TRP	1737	28.080	-3.113	2.248	1.00 20.57
ATOM	2459	CB	TRP	1737	29.107	-2.682	3.291	1.00 17.02
ATOM	2460	CG	TRP	1737	28.558	-2.415	4.654	1.00 20.35
ATOM	2461	CD2		1737	29.254	-2.564	5.897	1.00 20.42
ATOM	2462	CE2		1737	28.387	-2.122	6.923	1.00 21.18
ATOM	2463	CE3		1737	30.538	-3.027	6.243	1.00 21.60
ATOM	2464	CD1		1737	27.317	-1.914	4.970	1.00 19.86
ATOM	2465	NE1		1737	27.210	-1.732	6.328	1.00 21.03
ATOM	2467		TRP	1737	28.760	-2.125	8.276	1.00 21.70
ATOM	2468		TRP	1737	30.910	-3.031	7.594	1.00 21.73
ATOM	2469	CH2	TRP	1737	30.025	-2.584	8.588	1.00 23.06



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ATOM	2534	CZ	ARG	1744	24.592	-1.201	-1.663	1.00 22.92
MOTA	2535	NH1	ARG	1744	23.332	-0.814	-1.458	1.00 18.28
ATOM	2538		ARG	1744	25.491	-0.310	-2.060	1.00 22.15
MOTA	2541	C	ARG	1744	23.163		-1.833	1.00 24.61
ATOM	2542	0	ARG	1744	22.428	-8.755	-2.786	1.00 26.94
MOTA	2543	N	PRO	1745	23.143	-9.155	-0.688	1.00 23.21
ATOM	2544	CD	PRO	1745	24.052	-9.107	0.470	1.00 22.38
MOTA	2545	CA	PRO	1745	22.129	-10.190	-0.522	1.00 22.24
MOTA	2546	CB	PRO	1745	22.623	-10.942	0.711	1.00 21.13
MOTA	2547	CG	PRO	1745	23.286	-9.864	1.504	1.00 20.24
ATOM	2548	C	PRO	1745	20.800	-9.506	-0.256	1.00 23.11
ATOM	2549	0	PRO	1745	20.743	-8.300	0.020	1.00 25.93
ATOM	2550	N	THR	1746	19.724	-10.256	-0.373	1.00 20.82
ATOM	2552	CA	·THR	1746	18.420	-9.697	-0.112	1.00 20.47
ATOM	2553	CB	THR	1746	17 386	-10.342	-1.041	1.00 18.61
MOTA	2554	OG1		1746	17.382	-11.755	-0.822	1.00 21.86
MOTA	2556	CG2		1746	17.746	.10.078	-2.487	1.00 21.13
ATOM	2557	C	THR	1746	18.060	-9.970	1.344	1.00 20.84
ATOM	2558	0	THR	1746	18.787	-10.674	2.055	1.00 22.08
ATOM	2559	N	PHE	1747	16.953	-9.406	1.810	1.00 21.58
MOTA	2561	CA	PHE	1747	16.536	-9.675	3.178	1.00 21.15
ATOM	2562	CB	PHE	1747	15.442	-8.710	3.613	1.00 20 34
ATOM	2563	CG	PHE	1747	15.961	··7.350	3.982	1.00 23.18
ATOM	2564	CD1		1747	16.729	-7 170	5.130	1.00 22.26
ATOM	2565	CD2		1747	15.668	-6.240	3.196	1.00 23.41
ATOM	2566	CE1		.1747	17.186	-5.909	5.484	1.00 17.31
ATOM	2567	CE2	PHE	1747	15.124	-4.967	3.548	1.00 17.93
ATOM	2568	CZ	PHE	1747	16.883	-4.809	4.696	1.00 19.06
ATOM	2569	С	PHE	1747	16.062	-11.124	3.217	1.00 21.61
ATOM	2570	0	PHE	1747		-11.823	4.212	1.00 22.19
ATOM	2571	И	LYS	1748		-11.588	2.111	1.00 22.00
ATOM	2573	CA	LYS	1748		-12.973	2.009	1.00 24.34
ATOM	2574	CB	LYS	1748		-13.227	0.621	1.00 23.61
ATOM	2575	CG	LYS	1748		-14.663	0.416	1.00 27.45
MOTA.	2576	CD	LYS	1748		-14.932	-0.998	1.00 28.97
ATOM	2577	CE	LYS	1748		-16.394	-1.163	1.00 35.95
ATOM ATOM	2578	NZ	LYS	1748		-16.795	-0.153	1.00 41.69
ATOM	2582	C C	LYS	1748		-13.907	2.264	1.00 27.58
ATOM	2583 2584	N	LYS	1748		-14.863	3.034	1.00 29.73
ATOM	2586	CA	GLN GLN	1749		-13.604	1.640	1.00 25.88
ATOM	2587	CB	GLN	1749 1749		-14.394 -13.925	1.804	1.00 23.72
ATOM	2588	CG	GLN	1749			0.837	1.00 27.00
ATOM	2589	CD	GLN	1749		-13.954	-0.628	1.00 32.28
ATOM	2590					-13.331	-1.477	1.00 36.35
ATOM	2591	OE1 NE2	GLN	1749 1749		-12.528	-2.368	1.00 37.63
ATOM	2591 2594	NE2	GLN	1749		-13.702	-1.194	1.00 38.60
ATOM	2594 2595	0	GLN			-14.266	3.212	1.00 23.44
ATOM	2595 2596	N	LEU	1749 1750		-15.260 -13.035	3.826	1.00 23.52
ATOM	2598	CA	LEU	1750			3.703	1.00 21.73
MOTA	2599	CB	LEU	1750		-12.796 -11.308	5.054	1.00 20.90
ATOM	2600	CG	LEU	1750		-11.308	5.359	1.00 18.60
-11 OF	2000	CG	1150	1/30	20.654	-10.439	4.485	1.00 16.53

2.0	70		
	TOM 2601 CD	1 LEU 1750	20.190 -8.979 4.570
	TOM 2602 CD	2 LEU 1750	22 100 15.979 4.579 1.00 13.28
	1OM 2603 C	LEU 1750	10.012 4 939 1 00
	TOM 2604 O	LEU 1750	10.5348 6.108 1.00 21.25
	OM 2605 N	VAL 1751	7 084 1 00 0
	OM 2607 CA	VAL 1751	17.671 -13.607 5 917 1 00 05
	OM 2608 CB	VAL 1751	
TA	OM 2609 CG1	VAL 1751	14.0/2 6.432 1 00 20
AT	OM 2610 CG2	VAL 1751	14.453 -14.970 7.220 1.00 25
AT	OM 2611 C	• • • •	14.978 -12.648 6.684 1.00 25.34
ATO	OM 2612 O		17.127 -15.774 6 925 1 00 55
ATC	OM 2613 N		17.111 -16.369 8 007 1 00 55
ATC		~	17.418 -16.381 5 770 1 00 25.61
ATC		GLU 1752	17.773 -17.789 5 755 1 00
ATO	M 2617 CG	GLU 1752	17.765 -18.317 4 321 1 00 32.38
ATO		GLU 1752	16 799 30 37.26
ATO.		GLU 1752	16 394 -10 740
ATO			15 397 -18 405
АТО	M 252		17 377 -10 410
ATO	A 3037 (	GLU 1752	19.140 -17.00
ATOM	V 2522	GLU 1752	19 330 - 30 00-
ATOM	4 2625	ASP 1753	20 069 -17 006
ATOM	1 2626	ASP 1753	21 411 -12 124
ATOM	1 3620 -	ASP 1753	22 341 -16 144
ATOM	-02, CG /	ASP 1753	22 498 -16 355
ATOM	051 7	ASP 1753	22 222
ATOM	JD2 F	ISP 1753	22 908 -15 407 1.00 43.01
ATOM		SP 1753	21 379 76 225
	U M	SP 1753	31 071 8.153 1.60 33.84
ATOM	-002 M L	EU 1754	20 652 4-7/3 8.901 1.00 36.22
ATOM		EU 1754	20.560 8.633 1.00 30.73
ATOM		EU 1754	10.000 13.730 10.070 1.00 28.51
ATOM		EU 1754	20 010 14.394 10.355 1.00 25.20
ATOM	2637 CD1 L		20 045 25 10.016 1.00 26.72
ATOM	2638 CD2 L	EU 1754	27 020 24 18
ATOM	2639 C L		10.050 13.108 11.063 1.00 25 69
ATOM	2640 O LE		20.370 10.763 1.00 28.74
ATOM	2641 N AS		10 024 17.290 11.832 1.00 29.08
ATOM	2643 CA AS		10.130 1.00 29.97
ATOM	2644 CB AS		10.519 10.732 1 00 35 -
ATOM	2645 CG AS		
ATOM	2646 OD1 AS		16.100 -20.005 10 467 1 00 11
ATOM	2647 OD2 AS	P 1755	
ATOM	2648 C AS:		13.813 -20.995 9 774 1 22
ATOM	2649 O ASI		19.040 -19.703 10.952 1.00 33
ATOM	2650 N AR		18.9/8 -20.380 11 979 1 00 20
ATOM	2652 CA ARC		19.926 -19.923 9 989 1 00 55
ATOM	2653 CB ARG	_ <del></del>	20.884 -21.015 10.059 1.00 22.32
ATOM	2654 CG ARG		21.598 -21.145 8.704 1.00 32.73
ATOM	3655		22.733 -22.157 8.645 1.00 37 -
ATOM	2656		23.299 -22.274 7.237 1.00 37.78
ATOM	2650	• •	23.791 -20.999 6 702 1 00 43.87
ATOM		· -	24.890 -20.380 7 122 7 00 75
	2659 NH1 ARG	1756	25 630 20 01.
			23.030 -20.914 8.091 1.00 55.88
_			

MOTA	2662	NH2	ARG	1756	25.237	-19.214	6.593	1.00	52.53
MOTA	2665	С	ARG	1756	21.889	-20.761	11.186	1.00	33.76
MOTA	2666	0	ARG	1756	22.131	-21.619	12.049	1.00	34.53
ATOM	2667	N	ILE	1757	22.432	-19.553	11.204	1.00	33.49
MOTA	2669	CA	ILE	1757	23.405	-19.176	12.205	1.00	32.71
MOTA	2670	CB	ILE	1757	23.980	-17.764	11.919	1.00	31.86
ATOM	2671	CG2	ILE	1757	25.111	-17.454	12.869	1.00	31.71
ATOM	2672	CG1	ILE	1757	24.520	-17.704	10.488	1.00	31.41
MOTA	2673	CD1	ILE	1757	25.075	-16.366	10.096	1.00	27.68
MOTA	2674	С	ILE	1757	22.807	-19.236	13.604	1.00	34.20
MOTA	2675	0	ILE	1757	23.399	-19.833	14.495	1.00	35.83
MOTA	2676	N	VAL	1758	21.620	-18.667	13.792	1.00	35.40
MOTA	2678	CA.	VAL	1758	20.981	-18.653	15.108	1.00	37.49
MOTA	2679	CB	VAL	1758	19.501	-18.160	15.061	1.00	34.42
ATOM	2680	CG1	VAL	1758	18.899	-18.199	16.456	1.00	37.37
ATOM	2681	CG2	VAL	1758	19.403	-16.742	14.519	1.00	30.02
MOTA	2682	С	VAL	1758	21.010	-20.050	15.715	1.00	41.64
MOTA	2683	0	VAL	1758	21.533	-20.246	16.817	1.00	43.69
ATOM	2684	N	ALA	1759	20.492	-21.015	14 961	1.00	44.52
ATOM	2686	CA	ALA	1759	20.434	-22.415	15.387	1.00	45.20
MOTA	2687	CB	ALA	1759	19.833	-23.268	14.277	1.00	43.44
MOTA	2688	C	ALA	1759	21.7.91	-22.968	15.795	1.00	45.91
MOTA	2689	0	ALA	1759	21.890	-23.780	16.710	1.00	47.41
ATOM	2690	N	LEU	1760	22.833	-22.511	15.120	1.00	47.70
MOTA	2692	CA	LEU	1760	24.190	-22.960	15.399	1.00	50.91
ATOM	2693	CB	LEU	1760	25.015	-22.912	14.109	1.00	52.93
ATOM	2694	CG	LEU	1760	24.448	-23.723	12.947	1.00	57.55
MOTA	2695	CD1	LEU	1760 .	25.189	-23.390	11.660	1.00	60.76
ATOM	2696	CD2	LEU	1760	24.539	-25.208	13.273	1.00	58.66
ATOM	2697	C	LEU	1760	24.882	-22.111	16.472	1.00	52.07
ATOM	2698	O	LEU	1760	25.967	-22.459	16.953	1.00	51.95
ATOM	2699	N	THR	1761		-21.000	16.850	1.00	52.05
MOTA	2701	CA	THR	1761 .	24.868	-20.131	17.836	1.00	53.28
MOTA	2702	CB	THR	1761	24.362	-18.693	17.673	1.00	54.58
MOTA	2703	OG1	THR	1761	24.633	-18.259	16.339		53.68
ATOM	2705	CG2	THR	1761	25.090	-17.762	18.621	1.00	55.45
MOTA	2706	С	THR	1761	24.715	-20.619	19.272	1.00	53.31
ATOM	2707	0	THR	1761		-20.986	19.713	1.00	53.89
ATOM	2708	N	SER	1762		-20.617	19.993	1.00	53.51
ATOM	2710	CA	SER	1762		-21.045	21.383		53.15
ATOM	2711	CB	SER	1762		-21.131	21.830	1.00	57.27
MOTA	2712	OG	SER	1762		-21.872	23.028	1.00	61.22
ATOM	2714	С	SER	1762		-20.048	22.257	1.00	49.15
MOTA	2715	0	SER	1762	25.229	-18.831	22.071		46.61
ATOM	3466	N	ALA	461	79.636	26.047	14.493		61.05
MOTA	3468	CA	ALA	461	79.609	24.852	13.654	1.00	58.10
ATOM	3469	CB	ALA	461	78.335	24.024	13.935	1.00	60.39
MOTA	3470	C	ALA	461	79.694	25.239	12.179		54.65
ATOM	3471	0	ALA	461	79.653	24.382	11.297		54.05
ATOM	3472	N	ALA	462	79.867	26.537	11.935	1.00	51.68
ATOM	3474	CA	ALA	462	79.972	27.085	10.584	1.00	48.47
MOTA	3475	CB	ALA	462	80.099	28.619	10.633	1.00	46.99

ATO		476	C .	ALA	462	81.	123	26 40	0 0 0			
ATC		477	0	ALA	462	80.9		26.48 26.09			00 44.1	86
ATC		478	N '	ΓΥR	463	82.3					00 43.4	
ATO	-	180	CA :	ľYR	463	83.4		26.44			00 42.2	23
ATO		181	CB 7	YR	463	84.6		25.91	_		00 39.0	)4
ATO		82	CG 1	YR	463	84.3		26.92	_		00 39.0	)1
ATO		83	CD1 1	'YR	463	84.0		28.126			00 41.9	)5
ATO		84	CE1 T	YR	463	83.7		29.373			00 42.4	0
ATO		85	CD2 T	YR	463	84.3		30.466		12 1.	00 42.0	2
ATO		86	CE2 T	YR	463	83.9		28.009			00 40.7	
ATO		87 (	CZ T	YR	463	83.7		9.099			00 37.0	9
ATON		88 (	т но	YR	463	83.40		0.320		4 1.0	00 39.1	9
ATOM	-	90 (	T:	YR	463	84.0		1.406		0 1.0	0 40.66	6
ATOM		91 (		<b>r</b> R	463	84.62		4.554		0 1.0	0 37.78	3
ATOM		92 N			464			3.863		7 1.0	0 38.39	
ATOM		94 (	A GI		464	83.74		4.143		5 1.0	0 37.67	7
ATOM	349	95 C	B GI		464	84.21		2.841	11.74	7 1.0		
ATOM		6 C	G GL		464	85.70		2.890	12.02		0 41.44	
ATOM	349	7 C			464	86.09		3.870	13.10	3 1.0	0 47.87	
ATOM	349	8 0	E1 GL		164	87.58		1.135	13.169	9 1.0	0 53.44	
ATOM	349		E2 GL		164	87.99		1.983	13.990	1.0	0 56.72	
ATOM	350	0 C			64	88.34		3.513	12.397	7 1.00	54.85	
MOTA	350	1 0			64	83.50		.393	13.001	1.00	38.15	
ATOM	350	2 N			65	83.29		.187	13.905	1.00	39.59	
ATOM	3504	4 C.			65	83.123		.124	13.051	1.00	37.13	
MOTA	3509	5 CE			65	82.45		.608	14.236	1 00	37.93	
ATOM	350€	ce		_ •	65	81.502		.456	13.894	1.00	33.43	
ATOM	3507	CE	1 LEU		65	80.455		.609	12.787	1.00	31.12	
ATOM	3508				65	79.415		.500	12.944	1.00	24.85	
MOTA	3509	C	LEU	_	65	79.797		.980	12.855		29.05	
ATOM	3510	0	LEU		65	83.540		.090	15.166		41.02	
ATOM	3511	N	PRO		56	84.703		.93€	14.763		40.24	
ATOM	3512	CD	PRO		56	83.198		884	16.441		43.58	
ATOM	3513	CA				81.974		359	17.115	1.00	45.33	
ATOM	3514	CB	PRO	46		84.170		374	17.415		44.72	
ATOM	3515	CG	PRO	46		83.433			18.743		46.18	
ATOM	3516	C	PRO	46		82.486			18.496	1.00	48.84	
ATOM	3517	0	PRO	46		84.447	17.		17.101	1.00	44.52	
ATOM	3518	N	GLU	46		83.616	17.		16.509	1.00	43.38	
ATOM	3520	CA	GLU	46		85.610	17.		17.492	1.00	47.75	
ATOM	3521	CB	GLU	46		85.932	16.		17.218	1.00		
ATOM	3522	CG	GLU	46		87.354	15.		16.659	1.00	56.11	
ATOM	3523	CD	GLU	46		87.615	14.5		16.000	1.00	62.27	
ATOM	3524	OE1	GLU	46		88.927	14.4		15.242	1.00	66.39	
ATOM	3525		GLU	46		89.688	15.4		15.243	1.00	59.85	
ATOM	3526	C	GLU	46		89.182	13.4		4.643	1.00	56.09	
ATOM	3527	0	GLU	461		85.749	15.1		.8.435	1.00	19.62	
MOTA	3528	N	ASP	468		85.767	15.6		9.578	1.00 4	9.62	
ATOM	3530	CA	ASP	468		85.516	13.8		8.166	1.00 4		
ATOM	3531	CB	ASP			85.352	12.8	43 1		1.00 4	6.32	
ATOM	3532	CG	ASP	468		83.880	12.6	79 1		1.00 4		
ATOM	3533	OD1		468		83.678	11.7	40 2		1.00 4	4.19	
	_		- 1L) E	468		82.544	11.7			1.00 4		
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ATOM	3534	OD2	ASP	468	84.629	11.033	21.188	1.00	38.14
MOTA	3535	С	ASP	468	85.877	11.556	18.580	1.00	45.54
MOTA	3536	0	ASP	468	85.141	10.815	17.928	1.00	45.94
ATOM	3537	N	PRO	469	87.181	11.308	18.732	1.00	45.89
ATOM	3538	CD	PRO	469	88.111	12.189	19.464	1.00	45.11
ATOM	3539	CA	PRO	469	87.885	10.130	18.215	1.00	45.91
ATOM	3540	CB	PRO	469	89.208	10.187	18.968	1.00	45.90
ATOM	3541	CG	PRO	469	89.456	11.662	19.042	1.00	45.73
ATOM	3542	C	PRO	469	87.170	8.806	18.473	1.00	45.48
ATOM	3543	0	PRO	469	87.188	7.905	17.629	1.00	46.83
MOTA	3544	N	ARG	470	86.495	8.717	19.613	1.00	42.12
ATOM	3546	CA	ARG	470	85.786	7.506	19.999	1.00	41.21
MOTA	3547	CB	ARG	470	85.083	7.704	21.331	1.00	43.14
MOTA	3548	CG	ARG	470	85.885	8.424	22.375	1.00	45.68
ATOM	3549	CD	ARG	470	85.014	8.705	23.564	1.00	45.98
ATOM	3550	NE	ARG	470	83.802	9.417	23.184	1.00	47.28
MOTA	3552	CZ	ARG	470	82.921	9.877	24.057	1.00	50.54
MOTA	3553	NH1	ARG	470	83.127	9.687	25.354	1.00	47.56
ATOM	3556	NH2	ARG	470	81.843	10.527	23 637	1.00	54.59
ATOM	3559	С	ARG	470	84.736	7.058	19.004	1.00	40.57
ATOM	3560	0	ARG	470	84.411	5.877	18.941	1.00	43.13
ATOM	3561	14	TRP	471	84.182	8.014	18.268	1.00	38.07
ATOM	3563	C:A	TRP	471	83.124	7.736	17.314	1.00	35.09
MOTA	3564	CB	TRP	471	81.890	8.515	17.739	1.00	33.42
MOTA	3565	CG	TRP	471	81.259	7.958	18.952	1.00	31.71
ATOM	3566	CD2	TRP	471	80.512	6.740	19.026	1.00	34.81
MOTA	3567	CE2	TRP	471	80.061	6.610	20.355	1.00	33.17
ATOM	3568	CE3	TRP	471	80.174	5.744	18.092	1.00	37.60
MOTA	3569	CD1	TRP	471	81.246	8.503	20.199	1.00	25.70
MOTA	3570	NE1	TRP	471	80.525	7.697	21.051	1.00	28.79
MOTA	3572	CZ2	TRP	471	79.289	5.522	20.776	1.00	35.80
ATOM	3573	CZ3	TRP	471	79.409	4.660	18.509	1.00	35.52
MOTA	3574	CH2	TRP	471	78.973	4.560	19.839	1.00	34.51
ATOM	3575	C	TRP	471	83.432	8.065	15.872	1.00	35.77
ATOM	3576	0	TRP	471	82.690	7.670	14.968	1.00	37.45
ATOM	3577	N	GLU	472	84.533	8.770	15.651	1.00	34.76
ATOM	3579	CA	GLU	472	84.895	9.184	14.308		34.51
ATOM	3580	CB	GLU	472	86.065	10.174	14.365	1.00	32.30
MOTA	3581	CG	GLU	472	86.221	11.038	13.103	1.00	36.57
ATOM	3582	CD	GLU	472	85.082	12.035	12.872		36.34
ATOM	3583	OE1		472	84.515	12.558	13.857		36.01
ATOM	3584	OE2		472	84.777	12.318	11.694	1.00	31.95
ATOM	3585	C	GLU	472	85.219	8.034	13.364	1.00	33.90
MOTA	3586	0	GLU	472	85.896	7.082	13.745		33.77
MOTA	3587	N	LEU	473	84.667	8.094	12.158	1.00	33.58
ATOM	3589	CA	LEU	473	84.944	7.095	11.146	1.00	
MOTA	3590	CB	LEU	473	83.714	6.234	10.847	1.00	
ATOM	3591	CG	LEU	473	84.020	5.091	9.867	1.00	
MOTA	3592	CD1		473	84.786	4.000	10.578	1.00	
MOTA	3593	CD2		473	82.759	4.518	9.273	1.00	35.34
ATOM	3594	С	LEU	473	85.380	7.828	9.883	1.00	37.95
MOTA	3595	0	LEU	473	84.720	8.781	9.457	1.00	39.55

A'	TOM 3	596 N	_						
	_			74	86.	522	7 422		
		597 CD	PRO 4	74	87.		7.423	9.299	1.00 38.99
	- ·	598 CA	PRO 4	74	87.		6.453	9.899	1.00 38.76
		599 CB	PRO 4	4	07.0		8.004	8.080	1.00 39.37
		00 CG	PRO 47		88.3	_	7.201	7.906	1.00 40.18
		01 C	PRO 47		88.7		.883	9.310	1.00 37.76
		02 0	PRO 47		86.1	.65 7		6.890	1.00 37.76
AT		03 N	ARG 47		85.8	65 6		5.532	1.00 40.94
ATO		05 CA	800		85.7	62 g		5.245	1.00 43.98
ATO		0~			84.8	50 g		.101	1.00 40.66
ATO	OM 360	22			84.7	76 10	_	.448	1.00 40.66
ATC	OM 360				84.3				1.00 37.94
ATC			ARG 475		84.34			.415	1.00 36.12
ATO		1	ARG 475		83.93		<u> </u>	.800	1.00 35.92
ATO			ARG 475		82.67	-	<b>-</b>	.801	1.00 30.14
ATO			ARG 475		81.68			.170	1.00 28.45
ATO					82.41			.599	1.00 28.41
ATO			RG 475		85.14			197	1.00 27.85
ATON			RG 475		84.22			046 ]	.00 41.44
ATOM			SP 476		86.41		189 3.	470 I	.00 41.40
ATOM			SP 476		86.836		475 3.	830 1	.00 44.99
			SP 476		00.036		177 2.	849 1	.00 50.62
ATOM	2024		SP 476		88.344	-	540 2.		.00 54.47
ATOM			SP 476		89.105		69 3		.00 60.03
ATOM		OD2 AS	SP 476		89.569	-	10 3.		.00 65.09
ATOM		C AS	_		89.216		69 4.8		.00 62.62
ATOM	3628	O AS	- , 0		36.436		54 3.2		00 51.16
ATOM	3629	N AR	- , 0		36.678	4.0	91 2.5		00 51.16
ATOM	3631	CA AR	-,,	5	5.900	4.9	16 4.4		00 53.06
ATOM	3632	CB AR		8	5.443	3.62	23 4.9		00 49.58
ATOM	3633	CG AR			6.040	3.35			00 17.34
ATOM	3634	CD AR			7.481	2.92			00 48.85
ATOM	3635	NE ARO		8	8.169	3.07			00 52.11
ATOM	3637	CZ ARC		8	7.515	2.34			00 53.63
ATOM	3638	NH1 ARG		8.	7.932	2.36			00 54.86
ATOM	3641	NH2 ARG		89	9.000	3.07			00 57.15
ATOM	3644			87	7.269	1.69	-		00 55.98
ATOM	3645				.915	3.56		-	0 58.31
ATOM	3646				.339	2.78			0 44.70
MOTA	3648	N LEU		83	. 274	4.366			0 44.63
ATOM	3649	CA LEU	478	81	. 832	4.440			0 41.95
ATOM	200	CB LEU	478		.374				0 38.58
ATOM		CG LEU	478	79	. 872	5.609		1.0	0 33.17
ATOM		CD1 LEU	478	79	. 393	5.731		1.00	29.07
ATOM		CD2 LEU	478		590	4.592		1.00	28.25
ATOM		C LEU	478	81	432	7.059		1.00	30.79
ATOM		D LEU	478	81	938	4.710	2.674	1.00	38.93
ATOM		VAL.	479	an	562	5.647	2.071	1.00	41.75
		CA VAL	479			3.880	2.107		37.96
ATOM		B VAL	479		113	4.086	0.730		37.87
T mass	3659 C	G1 VAL	479	80.		2.882	-0.192	1.00	36.47
ATOM	3660 C	G2 VAL	479	80.		3.145	-1.612	1 00	34.43
	3661 C		479	81.		2.651	-0.187	1 00	34.43
ATOM	3662 O		479	78.6		4.299	0.775	1 00	34.33
			113	77.8	346	3.366	1.019	1 00	38.10 40.13
SSSD/5514								~.50	40.T3

MOTA	3663	N	LEU	480	78.184	5.537	0.552	1.00 38.05
ATOM	3665	CA	LEU	480	76.766	5.879	0.606	1.00 35.90
MOTA	3666	CB	LEU	480	76.568	7.393	0.475	1.00 33.98
ATOM	3667	CG	LEU	480	77.276	8.257	1.536	1.00 32.84
ATOM	3668	CD1	LEU	480	77.003	9.749	1.273	1.00 29.68
ATOM	3669	CD2	LEU	480	76.828	7.861	2.943	1.00 26.03
ATOM	3670	C	LEU	480	76.015	5.146	-0.476	1.00 34.99
ATOM	3671	0	LEU	480	76.573	4.864	-1.526	1.00 36.12
ATOM	3672	N	GLY	481	74.753	4.836	-0.223	1.00 35.21
ATOM	3674	CA.	GLY	481	73.965	4.120	-1.204	1.00 34.79
ATOM	3675	C	GLY	481	72.544	4.608	-1.332	1.00 36.31
ATOM	3676	0	GLY	481	72.237	5.775	-1.046	1.00 38.30
ATOM	3677	N	LYS	482	71.665	3.705	-1.761	1.00 35.59
ATOM	3679	CA	LYS	482	70.257	4.007	-1.959	1.00 35.24
MOTA	3680	CB	LYS	482	69.488	2.698	-2.207	1.00 35.69
MOTA	3681	C	LYS	482	. 69.585	4.763	-0.823	1.00 36.31
ATOM	3682	0	LYS	482	69.752	4.421	0.352	1.00 34.90
ATOM	3683	N	PRO	483	68.787	5.786	-1.157	1.00 38.08
MOTA	3684	CD	PRO	483	68.432	6.320	-2.483	1.00 39.57
MOTA	3685	CA	PRO	483	68.097	6.566	-0.135	1.00 41.08
A'TOM	3686	CB	PRO	483	67.300	7.560	-0.987	1.00 39.80
ATOM	3687	CG	PRO	483	68.268	7.819	-2.157	1.00 37.87
MOTA	3688	C	PRO	483	67.130	5.652	0.606	1.00 42.11
ATOM	3689	0	PRO	483	66.306	1.994	-0.025	1.00 43 01
A.TOM	3690	11	LEU	484	67.199	5.624	1.937	1.00 41.06
MOTA	3692	CA	LEU	484	66.293	4.823	2.751	1.00 38.47
ATOM	3693	CB	LEU	484	67.040	4.307	3.990	1.00 32.45
MOTA	3694	CG	LEU	484	67.968	3.098	3.809	1.00 27.68
ATOM	3695	CD1	LEU	484	68.569	2.710	5.147	1.00 20.29
ATOM	3696	CD2	LEU	484	67.181	1.964	3.225	1.00 23.20
ATOM	3697	С	LEU	484	65.084	5.637	3.180	1.00 42.18
MOTA	3698	O	LEU	484	65.227	6.699	3.814	1.00 44.50
ATOM	3699	14	GLY	485	63.893	5.170	2.817	1.00 45.68
MOTA	3701	CA	GLY	485	62.692	5.863	3.220	1.00 49.88
ATOM	3702	C	GLY	485	62.216	7.008	2.337	1.00 53.01
MOTA	3703	O	GLY	485	62.438	7.005	1.117	1.00 50.26
MOTA	3704	N	GLU	486	61.592	8.020	2.949	1.00 56.24
ATOM	3706	CA	GLU	486	61.064	9.183	2.257	1.00 58.07
ATOM	3707	CB	GLU	486	59.666	8.845	1.682	1.00 55.60
MOTA	3708	C	GLU	486	60.995	10.477	3.088	1.00 59.35
ATOM	370 <del>9</del>	0	GLU	486	60.019	11.226	3.000	1.00 61.44
MOTA	3710	N	GLY	487	62.027	10.747	3.879	1.00 59.60
ATOM	3712	CA	GLY	487	62.066	11.964	4.652	1.00 59.75
MOTA	3713	C	GLY	487	61.337	11.959	5.974	1.00 61.44
ATOM	3714	0	GLY	487	61.231	12.979	6.627	1.00 61.96
ATOM	3715	N	ALA	488	60.820	10.800	6.377	1.00 59.69
ATOM	3717	CA	ALA	488	60.134	10.709	7.657	1.00 57.27
ATOM	3718	CB	ALA	488	59.489	9.337	7.825	1.00 58.05
ATOM	3719	С	ALA	488	61.137	10.970	8.754	1.00 56.28
MOTA	3720	Ο ·	ALA	488	60.810	11.446	9.834	1.00 57.31
ATOM	3721	N	PHE	489	62.389	10.630	8.480	1.00 54.40
ATOM	3723	CA	PHE	489	63.462	10.830	9.466	1.00 54.56

ATOM 3726 CB PHE 489 63.022 8.454 10.352 1.00 45.21 ATOM 3726 CCD PHE 489 63.027 8.344 10.352 1.00 43.48 ATOM 3727 CD2 PHE 489 63.057 7.585 9.516 1.00 43.48 ATOM 3728 CE1 PHE 489 63.057 7.585 9.516 1.00 43.48 ATOM 3728 CE2 PHE 489 63.057 8.344 11.736 1.00 35.02 ATOM 3730 CZ PHE 489 61.625 6.653 10.039 1.00 36.502 ATOM 3731 CZ PHE 489 61.433 6.558 11.407 1.00 34.79 ATOM 3732 O PHE 489 61.433 6.558 11.407 1.00 34.79 ATOM 3733 O PHE 489 65.372 12.276 9.692 1.00 59.05 ATOM 3733 O PHE 489 65.372 12.276 9.692 1.00 55.60 ATOM 3733 O PHE 489 65.372 12.276 9.692 1.00 55.60 ATOM 3735 CA GLV 490 65.899 12.778 5.993 1.00 55.66 ATOM 3737 O GLV 490 65.899 12.778 5.993 1.00 55.60 ATOM 3737 O GLV 490 65.899 12.778 5.993 1.00 55.60 ATOM 3734 O GLV 490 65.899 12.778 5.993 1.00 55.60 ATOM 3734 O GLV 490 65.899 12.778 5.993 1.00 55.60 ATOM 3740 CA GLN 491 67.033 13.304 5.634 1.00 53.44 ATOM 3741 CB GLN 491 67.033 13.304 5.634 1.00 53.44 ATOM 3742 CG GLN 491 67.033 13.304 5.634 1.00 53.44 ATOM 3744 CB GLN 491 69.762 12.818 5.265 1.00 57.10 ATOM 3744 OC GLN 491 69.762 12.818 5.265 1.00 57.10 ATOM 3744 OC GLN 491 69.669 11.704 5.805 1.70 57.49 ATOM 3748 C GLN 491 70.045 13.082 0.441 1.00 62.79 ATOM 3748 C GLN 491 70.045 13.082 0.441 1.00 62.78 ATOM 3755 C VAL 492 68.705 9.093 5.456 1.00 46.97 ATOM 3755 C VAL 492 68.705 9.093 5.456 1.00 46.97 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 46.97 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 46.97 ATOM 3757 C VAL 492 68.705 9.093 5.456 1.00 46.97 ATOM 3760 C VAL 493 70.506 7.800 3.158 1.00 43.75 ATOM 3760 C VAL 493 71.608 7.471 2.148 1.00 45.61 ATOM 3760 C VAL 493 71.608 7.471 2.148 1.00 45.61 ATOM 3760 C VAL 493 71.608 7.471 2.148 1.00 45.61 ATOM 3760 C VAL 493 71.608 7.472 2.148 1.00 46.62 ATOM 3760 C VAL 493 71.608 7.472 2.148 1.00 46.70 ATOM 3776 C VAL 493 71.608 7.472 2.148 1.00 46.70 ATOM 3777 C G LEU 494 71.609 2.158 3.158 3.142 1.00 43.73 ATOM 3760 C VAL 493 71.608 7.472 2.148 1.00 46.68 ATOM 3778 C C VAL 493 71.609 2.268 3.499 1.00 43.75 ATOM 3779 C C LEU 494 71.609 2.004 3.159 1.00	<b>&gt;</b>	
ATOM 3725 CG PHE 489 63.222 8.454 10.352 1.00 49.88 ATOM 3726 CD1 PHE 489 62.505 7.585 9.516 1.00 43.48 ATOM 3727 CD2 PHE 489 62.505 7.585 9.516 1.00 43.48 ATOM 3728 CE1 PHE 489 61.625 6.653 10.09 1.00 36.69 ATOM 3729 CD2 PHE 489 61.625 6.653 10.09 1.00 36.69 ATOM 3730 CZ PHE 489 61.433 6.558 11.407 1.00 35.02 ATOM 3731 C PHE 489 61.433 6.558 11.407 1.00 35.02 ATOM 3732 O PHE 489 61.433 6.558 11.407 1.00 35.02 ATOM 3735 CA GLY 490 65.372 12.276 9.692 1.00 59.05 ATOM 3736 C GLY 490 65.372 12.276 9.692 1.00 59.05 ATOM 37376 C GLY 490 65.899 12.778 5.993 1.00 55.60 ATOM 3737 CA GLY 490 65.357 11.854 5.366 1.00 54.79 ATOM 3738 N GLM 491 65.357 11.854 5.366 1.00 54.79 ATOM 3741 CB GLN 491 67.073 13.304 5.634 1.00 53.44 ATOM 3741 CB GLN 491 67.073 13.304 5.634 1.00 53.44 ATOM 3743 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3743 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3743 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.05 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 59.19 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 46.38 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 46.38 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 46.97 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 47.93 ATOM 3756 C VAL 492 68.103 10.318 4.984 1.00 47.93 ATOM 3756 C VAL 492 68.103 10.318 4.984 1.00 47.93 ATOM 3756 C VAL 492 68.103 10.318 4.984 1.00 47.93 ATOM 3756 C VAL 493 71.568 7.471 2.148 1.00 47.93 ATOM 3756 C VAL 493 71.568 7.471 2.148 1.00 43.75 ATOM 3766 C VAL 493 71.568 7.492 68.103 10.318 4.984 1.00 44.71 ATOM 3766 C VAL 493 71.568 7.492 68.181 7.00 40.00 40.80 40.70 40.70 40.70 40.70 40.70 40.70 40.70 40.70 40.70 40.70 40.7	CD PRE 480	
ATOM 3726 CD1 PHE 489 63.017 8.344 10.352 1.00 45.21 ATOM 3728 CE1 PHE 489 63.017 8.344 11.738 1.00 40.99 ATOM 3729 CE2 PHE 489 61.625 6.653 10.039 1.00 36.69 ATOM 3731 C PHE 489 61.625 6.653 10.039 1.00 36.69 ATOM 3731 C PHE 489 61.625 6.653 10.039 1.00 36.69 ATOM 3731 C PHE 489 61.625 6.653 10.039 1.00 36.69 ATOM 3731 C PHE 489 61.433 6.558 11.407 1.00 34.73 ATOM 3732 C PHE 489 61.433 6.558 11.407 1.00 34.73 ATOM 3733 N GLY 490 64.456 11.896 8.974 1.00 56.31 ATOM 3735 CA GLY 490 65.899 12.778 5.993 1.00 55.31 ATOM 3737 C GLY 490 65.899 12.778 5.993 1.00 55.60 ATOM 3737 C GLY 490 65.899 12.778 5.993 1.00 55.60 ATOM 3740 CA GLN 491 67.073 13.304 5.366 1.00 57.10 ATOM 3741 CB GLN 491 67.073 13.304 5.366 1.00 57.10 ATOM 3741 CB GLN 491 67.073 13.304 5.366 1.00 57.10 ATOM 3742 CG GLN 491 68.760 13.580 3.777 1.00 53.44 ATOM 3743 CD GLN 491 69.669 12.658 4.562 1.00 57.19 ATOM 3740 CB GLN 491 70.046 13.566 1.00 57.19 ATOM 3740 CB GLN 491 70.046 13.566 1.00 57.19 ATOM 3740 CB GLN 491 70.046 13.566 4.562 1.00 57.19 ATOM 3740 CB GLN 491 70.046 13.566 4.562 1.00 57.19 ATOM 3740 CB GLN 491 70.046 13.566 5.634 1.00 53.44 ATOM 3749 CB GLN 491 70.045 13.560 3.777 1.00 53.48 ATOM 3750 N VAL 492 68.705 9.093 5.456 1.00 49.56 ATOM 3752 CA VAL 492 68.705 9.093 5.456 1.00 49.56 ATOM 3755 CG2 VAL 492 68.705 9.093 5.456 1.00 49.89 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 49.89 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 46.70 ATOM 3766 CA VAL 493 71.506 7.471 1.00 52.79 ATOM 3766 CA VAL 493 71.506 7.471 1.00 44.71 1.00 42.79 ATOM 3766 CA VAL 493 71.506 7.471 1.00 44.71 1.00 42.79 ATOM 3766 CA VAL 493 71.506 7.471 1.00 43.73 ATOM 3766 CA VAL 493 71.506 7.471 1.00 43.73 ATOM 3766 CA VAL 493 71.506 7.471 1.00 43.73 ATOM 3767 CB LEU 494 71.100 7.100 7.100 41.79 ATOM 3777 CB LEU 494 71.609 0.001 3.860 1.00 43.79 ATOM 3767 CB LEU 494 71.609 0.001 3.860 1.00 43.79 ATOM 3768 CB LEU 494 71.609 0.001 3.860 1.00 43.79 ATOM 3778 CB LEU 494 71.609 0.001 3.800 1.00 44.71 1.00 45.23 ATOM 3779 C	ATUM 3725 CG DUE	9.500 9.770
ATOM 3727 CD2 PHE 489 62.505 7.585 9.516 1.00 43.48 ATOM 3728 CE2 PHE 489 61.625 6.653 10.09 10.09 10.00 36.69 ATOM 3730 CZ PHE 489 61.625 6.653 10.09 10.00 36.69 ATOM 3731 C PHE 489 61.433 6.558 11.407 10.0 35.02 ATOM 3731 C PHE 489 61.433 6.558 11.407 10.00 34.73 ATOM 3732 O PHE 489 61.433 6.558 11.407 10.00 34.73 ATOM 3733 N GLV 490 65.372 12.276 9.692 10.0 55.05 ATOM 3736 C GLV 490 65.372 12.276 9.692 10.0 55.05 ATOM 3736 C GLV 490 65.811 13.400 7.143 1.00 55.60 ATOM 3737 N GLV 490 65.899 12.778 5.993 10.0 54.79 ATOM 3738 N GLN 491 65.899 12.778 5.993 10.0 54.79 ATOM 3741 CB GLN 491 67.073 13.304 5.634 10.0 53.44 ATOM 3741 CB GLN 491 67.073 13.304 5.634 10.0 53.44 ATOM 3742 CG GLN 491 66.760 13.580 3.777 1.00 53.48 ATOM 3748 NEZ GLN 491 70.046 13.696 1.548 1.00 53.48 ATOM 3749 O GLN 491 70.046 13.696 1.00 57.19 ATOM 3748 CB GLN 491 70.453 13.062 0.441 1.00 53.48 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 62.09 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 63.78 ATOM 3755 CS VAL 492 68.103 10.318 4.984 1.00 63.78 ATOM 3755 CV VAL 492 68.103 10.318 4.984 1.00 63.78 ATOM 3756 C VAL 492 68.103 10.318 4.984 1.00 63.78 ATOM 3757 O VAL 492 68.103 10.318 4.984 1.00 64.79 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 46.38 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.71 ATOM 3766 C VAL 493 70.200 7.654 1.00 43.73 ATOM 3766 C VAL 493 70.200 7.654 1.00 43.73 ATOM 3766 C VAL 493 70.200 7.654 1.00 43.73 ATOM 3766 C VAL 493 70.200 7.654 1.00 43.73 ATOM 3766 C VAL 493 70.200 7.654 1.00 43.73 ATOM 3766 C VAL 493 71.508 7.428 2.706 1.00 43.73 ATOM 3766 C VAL 493 71.508 7.428 2.706 1.00 43.73 ATOM 3766 C VAL 493 71.608 7.417 2.148 1.00 46.20 ATOM 3777 C LEU 494 71.608 7.429 1.00 43.73 ATOM 3766 C VAL 493 71.608 7.417 2.148 1.00 43.73 ATOM 3766 C VAL 493 71.608 7.417 2.148 1.00 43.73 ATOM 3766 C VAL 493 71.608 7.417 2.148 1.00 43.73 ATOM 3767 C LEU 494 71.608 7.428 2.706 1.00 43.78 ATOM 3778 C BALA 495 76.699 1.00 2.725 1.00 42.72 ATOM 3779 C BALA 495 76.699 4.032 3.851 1.00 43.73 ATOM 3779 C BALA 495 76.617 1.566 8.88 4.955	ATUM 373C on	03.222 8.454 10 252
ATOM 3728 CEI PHE 489 61.625 6.653 10.039 1.00 40.99 ATOM 3730 CZ PHE 489 61.625 6.653 10.039 1.00 36.62 ATOM 3731 C PHE 489 61.435 6.558 11.407 1.00 35.62 ATOM 3732 O PHE 489 62.138 7.411 1.257 1.00 35.62 ATOM 3733 N GLY 490 65.372 12.276 9.692 1.00 59.05 ATOM 3735 CA GLY 490 65.891 12.375 7.735 1.00 55.60 ATOM 3737 O GLY 490 65.899 12.778 5.993 1.00 54.79 ATOM 3737 O GLY 490 65.899 12.778 5.993 1.00 54.79 ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 53.40 ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 53.40 ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 53.40 ATOM 3740 CB GLN 491 69.422 12.818 2.629 1.00 53.40 ATOM 3740 CB GLN 491 69.422 12.818 2.629 1.00 53.40 ATOM 3744 CB GLN 491 70.143 1.696 1.00 57.19 ATOM 3745 NE2 GLN 491 70.046 13.696 1.548 1.00 62.78 ATOM 3745 NE2 GLN 491 70.131 14.893 1.701 1.00 57.19 ATOM 3745 NE2 GLN 491 70.453 13.092 0.441 1.00 57.19 ATOM 3752 CA VAL 492 68.103 10.318 4.894 1.00 49.89 ATOM 3753 CB VAL 492 68.103 10.318 4.894 1.00 49.89 ATOM 3755 CC VAL 492 68.103 10.318 4.894 1.00 46.38 ATOM 3756 C VAL 492 68.103 10.318 4.894 1.00 46.38 ATOM 3756 C VAL 492 68.103 10.318 4.894 1.00 45.61 ATOM 3760 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3760 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3760 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3762 CG VAL 493 71.608 7.471 2.148 1.00 46.26 ATOM 3766 CB VAL 493 71.608 7.471 2.148 1.00 45.61 ATOM 3766 CB VAL 493 71.608 7.471 2.148 1.00 43.73 ATOM 3766 CB VAL 493 71.608 7.471 2.148 1.00 43.73 ATOM 3767 CB LEU 494 71.682 3.158 1.00 43.38 ATOM 3777 CD LEU 494 71.682 3.158 1.00 43.38 ATOM 3777 CD LEU 494 71.682 3.158 1.00 43.38 ATOM 3778 CB LEU 494 71.682 3.158 1.00 43.38 ATOM 3779 CB LEU 494 71.682 3.158 3.499 1.00 43.38 ATOM 3779 C B ALA 495 75.456 8.298 3.499 1.00 43.38 ATOM 3779 C B ALA 495 75.456 8.384 5.51 1.00 48.62 ATOM 3779 C B ALA 495 76.699 4.002 3.821 1.00 43.76 ATOM 3779 C B ALA 495 76.699 4.002 3.821 1.00 43.76 ATOM 3779 C B ALA 495 76.699 4.002 3.821 1.00 43.76 ATOM 3780 C B A	ATOM 2722	62.505 7.585 9.516 7.50 45.21
ATOM 3730 CE2 PHE 489 61.625 6.653 10.039 1.00 36.69 ATOM 3731 C PHE 489 62.138 7.411 12.257 1.00 35.02 ATOM 3732 C PHE 489 61.433 6.558 11.407 1.00 35.02 ATOM 3733 C PHE 489 65.372 12.276 9.692 1.00 59.03 ATOM 3733 N GLY 490 65.372 12.276 9.692 1.00 59.05 ATOM 3736 C GLY 490 65.141 13.400 7.143 1.00 55.60 ATOM 3737 N GLY 490 65.371 12.276 9.692 1.00 59.05 ATOM 3738 N GLN 490 65.371 12.276 9.692 1.00 59.05 ATOM 3738 N GLN 490 65.357 11.854 5.933 1.00 55.60 ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 57.10 ATOM 3741 CB GLN 491 67.073 13.304 5.634 1.00 57.10 ATOM 3742 CG GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3744 OE1 GLN 491 70.046 13.696 1.548 1.00 52.60 ATOM 3748 C GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3748 C GLN 491 70.453 13.082 0.441 1.00 62.09 ATOM 3749 O GLN 491 68.623 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.103 13.082 0.441 1.00 62.78 ATOM 3751 CB VAL 492 68.103 13.082 0.441 1.00 62.78 ATOM 3753 CB VAL 492 67.760 8.320 6.122 1.00 49.89 ATOM 3753 CB VAL 492 67.361 9.093 5.456 1.00 49.89 ATOM 3756 C VAL 492 67.361 9.01 3.580 1.00 49.89 ATOM 3756 C VAL 492 67.361 9.01 3.580 1.00 45.21 ATOM 3760 CA VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3760 CA VAL 493 70.596 6.780 3.109 1.00 45.71 ATOM 3760 CA VAL 493 70.596 6.780 3.109 1.00 44.71 ATOM 3760 CA VAL 493 70.596 6.780 3.109 1.00 44.71 ATOM 3760 CA VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3760 CG LVU 494 71.608 7.471 2.148 1.00 46.20 ATOM 3760 CG LVU 494 71.682 3.158 3.142 1.00 43.73 ATOM 3760 CG LVU 494 71.682 3.158 3.163 1.00 43.38 ATOM 3760 CG LVU 494 71.682 3.158 3.163 1.00 43.38 ATOM 3760 CG LVU 494 71.689 0.201 3.850 1.00 43.73 ATOM 3760 CG LVU 494 71.608 7.471 2.148 1.00 46.20 ATOM 3760 CG LVU 494 71.608 7.471 2.148 1.00 46.20 ATOM 3760 CG LVU 494 71.608 7.471 2.148 1.00 46.20 ATOM 3760 CG LVU 494 71.609 0.201 3.850 1.00 43.73 ATOM 3760 CG LVU 494 71.609 0.201 3.850 1.00 43.73 ATOM 3760 CG LVU 494 71.609 0.201 3.850 1.00 43.73 ATOM 3760 CG LVU 494 71.609 0.201 3.850 1.00 43.73 ATOM 3770 CG LEU 494 71.609 0.201 3.850 1.00 43.73 A	ATOM 3729 575	63.017
ATOM 3730 CZ PHE 489 62.138 7.411 12.257 1.00 35.02 ATOM 3731 C PHE 489 61.433 6.558 11.407 1.00 34.73 ATOM 3732 O PHE 489 64.456 11.896 8.974 1.00 55.02 ATOM 3733 N GLY 490 65.372 12.276 9.692 1.00 59.05 ATOM 3735 CA GLY 490 65.141 13.400 7.7143 1.00 59.05 ATOM 3737 C GLY 490 65.899 12.778 5.993 1.00 54.79 ATOM 3737 C GLY 490 65.899 12.778 5.993 1.00 54.79 ATOM 3740 CA GLN 491 67.073 13.304 5.636 1.00 54.79 ATOM 3740 CA GLN 491 67.073 13.304 5.636 1.00 54.79 ATOM 3741 CB GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3742 CG GLN 491 69.422 12.818 2.629 1.00 52.60 ATOM 3745 CG GLN 491 69.422 12.818 2.629 1.00 57.19 ATOM 3746 CG GLN 491 70.451 31.002 0.441 1.00 62.78 ATOM 3748 C GLN 491 70.453 13.002 0.441 1.00 62.78 ATOM 3750 N VAL 492 68.705 9.093 5.456 1.00 70.26 ATOM 3755 CG2 VAL 492 68.705 9.093 5.456 1.00 49.56 ATOM 3755 CG2 VAL 492 68.705 9.093 5.456 1.00 49.56 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 68.101 1.704 5.805 1.00 49.56 ATOM 3758 N VAL 493 70.210 7.654 4.208 1.00 45.23 ATOM 3750 N VAL 492 68.101 1.704 5.805 1.00 49.56 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 493 70.210 7.654 4.208 1.00 45.23 ATOM 3756 C VAL 493 70.210 7.654 4.208 1.00 45.23 ATOM 3756 C VAL 493 70.210 7.654 4.208 1.00 45.23 ATOM 3756 C VAL 493 70.210 7.654 4.208 1.00 45.23 ATOM 3756 C VAL 493 70.200 7.654 4.208 1.00 45.23 ATOM 3756 C VAL 493 70.200 7.654 4.208 1.00 43.75 ATOM 3757 N VAL 493 70.210 7.654 1.00 43.38 ATOM 3758 C LEU 494 71.608 7.471 2.148 1.00 43.38 ATOM 3757 N ALA 495 75.668 0.838 1.00 43.39 ATOM 3757 N ALA 495 75.668 0.838 1.500 4.752 1.00 43.75 ATOM 3777 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3778 C B LEU 494 71.609 -0.331 1.500 1.00 49.97 ATOM 3778 C B ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3779 C A ALA 495 75.668 0.838 4.551 1.00 49.79	ATOM 3729 CE2 700	61.625 6 653 11.738 1.00 40.99
ATOM 3731 C PHE 489 61.433 6.558 11.407 1.00 35.02 ATOM 3732 O PHE 489 64.456 11.896 8.974 1.00 56.31 ATOM 3733 N GLY 490 65.372 12.276 9.692 1.00 56.31 ATOM 3736 C GLY 490 65.372 12.276 9.692 1.00 56.05 ATOM 3737 N GLY 490 65.371 13.400 7.143 1.00 55.60 ATOM 3738 N GLN 490 65.357 11.854 5.993 1.00 55.60 ATOM 3738 N GLN 491 67.829 12.778 5.993 1.00 57.79 ATOM 3740 CA GLN 491 67.829 12.658 4.562 1.00 57.10 ATOM 3741 CD GLN 491 67.829 12.658 4.562 1.00 53.44 ATOM 3742 CG GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3744 CD GLN 491 69.422 12.818 2.629 1.00 53.48 ATOM 3745 NE2 GLN 491 70.046 13.696 1.548 1.00 53.48 ATOM 3745 NE2 GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3746 C GLN 491 70.453 13.082 0.441 1.00 62.09 ATOM 3750 N VAL 492 68.103 10.318 4.894 1.00 49.89 ATOM 3751 CD VAL 492 68.103 10.318 4.994 1.00 49.89 ATOM 3752 C VAL 492 68.103 10.318 4.994 1.00 46.38 ATOM 3756 C VAL 492 68.103 10.318 4.994 1.00 46.38 ATOM 3756 C VAL 492 68.103 10.318 4.994 1.00 46.70 ATOM 3756 C VAL 492 68.103 10.318 4.994 1.00 45.61 ATOM 3756 C VAL 492 68.103 10.318 4.994 1.00 45.61 ATOM 3758 N VAL 492 68.103 10.318 4.994 1.00 45.61 ATOM 3758 C VAL 492 68.103 10.318 4.994 1.00 45.61 ATOM 3756 C VAL 492 68.103 10.318 4.994 1.00 45.61 ATOM 3757 C C VAL 493 70.599 6.780 3.109 1.00 49.79 ATOM 3758 C C VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3758 C C VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3760 C A VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3760 C C VAL 493 71.608 7.471 ATOM 3761 C C VAL 493 71.608 7.471 ATOM 3762 C C VAL 493 71.608 7.471 ATOM 3763 C C VAL 493 71.608 7.471 ATOM 3760 C A VAL 493 71.608 7.471 ATOM 3761 C C VAL 493 71.608 7.471 ATOM 3762 C C VAL 493 71.608 7.471 ATOM 3763 C C VAL 493 71.608 7.471 ATOM 3760 C A VAL 493 71.608 7.471 ATOM 3760 C A VAL 493 71.608 7.471 ATOM 3760 C A VAL 493 71.608 7.471 ATOM 3761 C C VAL 493 71.608 7.471 ATOM 3760 C A VAL 493 71.608 7.471 ATOM 3760 C A VAL 493 70.599 6.780 3.199 1.00 49.79 ATOM 3770 C C LEU 494 70.600 -0.337 1.600 1.00 43.38 ATOM 3761 C B VAL 495 76.669 0.838 4.551 1.00	ATOM 3730 489	62.138 7.413
ATOM 3732 O PHE 489 64.456 11.896 8.974 1.00 56.31 ATOM 3733 N GLY 490 65.372 12.276 9.692 1.00 59.05 ATOM 3735 CC GLY 490 65.899 12.778 5.993 1.00 55.60 ATOM 3737 O GLY 490 65.899 12.778 5.993 1.00 55.60 ATOM 3737 O GLY 490 65.357 11.854 5.666 1.00 57.79 ATOM 3740 CA GLN 491 67.829 12.658 4.562 1.00 53.40 ATOM 3741 CB GLN 491 67.829 12.658 4.562 1.00 53.40 ATOM 3742 CG GLN 491 67.829 12.658 4.562 1.00 53.40 ATOM 3743 CD GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3744 CB GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3745 NE2 GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3748 C GLN 491 70.453 13.092 0.441 1.00 62.78 ATOM 3750 N VAL 492 68.632 11.518 5.165 1.00 49.89 ATOM 3751 CCZ VAL 492 68.705 9.093 5.456 1.00 47.83 ATOM 3752 CA VAL 492 68.705 9.093 5.456 1.00 47.83 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 47.83 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 46.97 ATOM 3756 CC VAL 492 68.103 10.318 4.984 1.00 47.83 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 68.103 10.318 4.984 1.00 47.93 ATOM 3756 C VAL 493 70.210 7.654 6.992 1.00 45.61 ATOM 3757 O VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3756 C VAL 493 70.210 7.654 6.992 1.00 45.61 ATOM 3756 C VAL 493 70.210 7.654 6.992 1.00 45.23 ATOM 3756 C VAL 493 70.210 7.654 1.00 43.75 ATOM 3756 C VAL 493 70.210 7.654 1.00 43.75 ATOM 3756 C LEU 494 71.608 7.471 2.148 1.00 43.75 ATOM 3756 C LEU 494 71.608 7.471 2.148 1.00 43.73 ATOM 3766 C A VAL 493 71.608 7.471 2.148 1.00 43.73 ATOM 3768 C LEU 494 71.608 2.330 2.366 1.00 43.38 ATOM 3767 C A LEU 494 71.609 0.201 3.850 1.00 43.73 ATOM 3776 C LEU 494 71.609 0.201 3.850 1.00 43.73 ATOM 3777 C A LEU 494 71.609 0.201 3.850 1.00 43.73 ATOM 3777 C A LEU 494 71.609 0.201 3.850 1.00 43.78 ATOM 3778 C B LEU 494 71.609 0.201 3.850 1.00 43.78 ATOM 3777 C A LA 495 75.668 0.838 4.551 1.00 43.78 ATOM 3778 C B LEU 494 71.609 0.201 3.850 1.00 43.78 ATOM 3779 C A ALA 495 75.668 0.838 4.551 1.00 43.78 ATOM 3779 C A ALA 495 75.668 0.838 4.551 1.00 49.79	ATOM 2727 - PHE 489	61 422 12.257 1.00 35.02
ATOM 3733 N GLY 490 65.372 12.276 9.692 1.00 59.05 ATOM 3735 CA GLY 490 65.899 12.778 5.993 1.00 56.56 1.00 56.56 ATOM 3736 N GLN 491 65.357 11.854 5.366 1.00 57.10 ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 55.60 ATOM 3741 CB GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3742 CG GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3744 OE1 GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3745 NE2 GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3745 NE2 GLN 491 70.046 13.696 1.500 62.09 ATOM 3745 NE2 GLN 491 70.045 13.082 1.500 62.09 ATOM 3755 N VAL 492 68.103 10.318 4.984 1.00 62.78 ATOM 3753 CB VAL 492 68.103 10.318 4.984 1.00 62.78 ATOM 3755 CG2 VAL 492 68.705 9.093 5.456 1.00 49.89 ATOM 3755 CG2 VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 46.70 ATOM 3758 N VAL 492 68.103 10.318 4.984 1.00 46.70 ATOM 3758 N VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 46.79 ATOM 3758 CG VAL 492 67.760 8.320 6.412 1.00 46.79 ATOM 3758 N VAL 492 68.103 10.318 4.984 1.00 46.70 ATOM 3758 N VAL 492 68.103 10.318 4.984 1.00 46.70 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3757 C VAL 493 70.599 6.780 3.099 1.00 44.71 ATOM 3760 CB VAL 493 70.599 6.780 3.099 1.00 44.71 ATOM 3760 CB VAL 493 70.599 6.780 3.099 1.00 44.71 ATOM 3760 CB VAL 493 70.599 6.780 3.099 1.00 44.71 ATOM 3761 CB VAL 493 70.599 6.780 3.099 1.00 43.78 ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 40.00 41.71 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 40.00 41.71 ATOM 3760 CB LEU 494 71.608 7.471 2.148 1.00 40.00 41.71 ATOM 3773 CD LEU 494 71.608 7.471 2.148 1.00 40.00 41.71 ATOM 3773 CD LEU 494 71.600 -0.337 T.760 1.00 43.78 ATOM 3770 CD LEU 494 71.600 -0.337 T.760 1.00 43.78 ATOM 3773 CD LEU 494 71.600 -0.337 T.760 1.00 43.78 ATOM 3773 CD L	ATOM 375 PHE 489	64 456 11 238 11.407 1.00 34.73
ATOM 3735 CA GLY 490 64.285 12.375 7.355 1.00 59.05   ATOM 3736 CA GLY 490 65.141 13.400 7.143 1.00 55.60   ATOM 3737 O GLY 490 65.899 12.778 5.993 1.00 54.79   ATOM 3738 N GLN 491 65.357 11.854   ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 57.10   ATOM 3741 CB GLN 491 67.073 13.304 5.634 1.00 57.10   ATOM 3742 CG GLN 491 68.760 13.580   ATOM 3743 CD GLN 491 69.422 12.818 2.629 1.00 52.60   ATOM 3745 NEZ GLN 491 70.046 13.696 1.548 1.00 62.09   ATOM 3746 C GLN 491 70.046 13.696 1.548 1.00 62.09   ATOM 3748 C GLN 491 68.632 11.518 5.165 1.00 49.89   ATOM 3750 N VAL 491 68.632 11.518 5.165 1.00 49.56   ATOM 3752 CA VAL 492 68.705 9.093 6.412 1.00 62.78   ATOM 3754 CG1 VAL 492 67.760 8.320 5.456 1.00 49.56   ATOM 3755 CG2 VAL 492 67.760 8.320 6.412 1.00 45.61   ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 45.61   ATOM 3757 O VAL 492 68.705 9.093 5.456 1.00 45.23   ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 45.61   ATOM 3763 CC VAL 493 70.210 7.655 4.208 1.00 45.23   ATOM 3760 CA VAL 493 70.210 7.654 4.208 1.00 45.75   ATOM 3761 CB VAL 493 70.210 7.654 4.208 1.00 45.75   ATOM 3763 CC2 VAL 493 71.608 7.471 2.148 1.00 46.20   ATOM 3766 N LEU 494 71.602 4.448 2.809 1.00 43.75   ATOM 3766 C VAL 493 71.608 1.548 1.00 46.16   ATOM 3767 CG LEU 494 71.609 -0.337 1.760 1.00 43.38   ATOM 3760 CA LEU 494 71.609 -0.337 1.760 1.00 43.38   ATOM 3761 CB LEU 494 71.609 -0.337 1.760 1.00 43.38   ATOM 3761 CB LEU 494 71.609 -0.337 1.760 1.00 43.38   ATOM 3763 CC2 VAL 493 71.608 2.3188 1.00 45.17   ATOM 3767 CA ALA 495 76.679 4.032 3.821 1.00 43.79   ATOM 3777 CA ALA 495 76.679 4.032 3.821 1.00 43.80   ATOM 3777 CA ALA 495 76.679 4.032 3.821 1.00 43.80   ATOM 3777 CA ALA 495 76.679 4.032 3.821 1.00 43.80   ATOM 3778 C ALA 495 76.679 7.330 1.288 2.090 1.00 43.80   ATOM 3778 C BLEU 494 71.568 0.338 1.309 1.00 43.80   ATOM 3778 C BLEU 494 71.568 0.338 1.309 1.00 43.80   ATOM 3778 C BLEU 494 71.568 0.338 1.309 1.00 43.80   ATOM 3778 C BLEU 494 71.568 0.338 1.00 43.80   ATOM 3778 C BLEU 494 71.689 0.201 3.850 1.00 43.80   ATOM 3778 C BL	ATOM 3735	65 272 10 8.974 1.00 56.31
ATOM 3736 C GLY 490 65.899 12.778 5.993 1.00 56.66 A ATOM 3737 C GLY 490 65.899 12.778 5.993 1.00 56.60 ATOM 3740 CA GLM 491 67.073 13.304 5.634 1.00 53.47 ATOM 3741 CB GLM 491 67.829 12.658 4.562 1.00 52.60 ATOM 3741 CB GLM 491 67.829 12.658 4.562 1.00 52.60 ATOM 3742 CG GLM 491 69.422 12.818 2.629 1.00 52.60 ATOM 3743 CD GLM 491 70.046 13.696 1.548 1.00 57.19 ATOM 3744 OEI GLM 491 70.046 13.696 1.548 1.00 57.19 ATOM 3748 C GLM 491 70.046 13.696 1.548 1.00 62.09 ATOM 3748 C GLM 491 70.453 13.082 0.441 1.00 62.78 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 62.78 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 49.66 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3755 CG VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3755 CG VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3756 C VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3757 O VAL 492 68.103 10.318 4.984 1.00 45.61 ATOM 3758 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 68.181 8.044 3.349 1.00 45.21 ATOM 3756 C VAL 493 70.509 6.780 3.109 1.00 45.21 ATOM 3760 CA VAL 493 70.509 6.780 3.109 1.00 45.21 ATOM 3760 CA VAL 493 70.509 6.780 3.109 1.00 45.21 ATOM 3760 CB VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CC VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CC VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CC VAL 493 71.608 7.471 2.148 1.00 43.73 ATOM 3760 CB LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3760 CB LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3761 CB LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3770 CG LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3770 CG LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3771 CD1 LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3773 C LEU 494 71.602 3.158 3.142 1.00 43.80 ATOM 3773 C LEU 494 71.602 3.158 3.142 1.00 43.80 ATOM 3773 C LEU 494 71.602 3.158 3.142 1.00 43.80 ATOM 3773 C LEU 494 71.602 3.158 3.142 1.00 43.8	N GLY 490	9.692 1 00 50 5-
ATOM 3737 C GIY 490 65.899 12.778 5.993 1.00 55.60 ATOM 3738 N GLN 491 65.357 11.854 5.366 1.00 57.10 ATOM 3740 CA GLN 491 67.829 12.658 4.562 1.00 53.44 ATOM 3741 CB GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3742 CG GLN 491 69.669 12.6818 2.629 1.00 57.19 ATOM 3743 CD GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3745 NE2 GLN 491 70.046 13.696 1.548 1.00 62.78 ATOM 3746 C GLN 491 68.632 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.705 9.093 5.456 1.00 49.89 ATOM 3750 CB VAL 492 68.705 9.093 5.456 1.00 47.83 ATOM 3750 CG VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 CC VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 493 70.510 7.654 4.208 1.00 43.75 ATOM 3760 CA VAL 493 70.510 7.654 4.208 1.00 43.75 ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 CA VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 CB LEU 494 71.692 8.000 2.366 1.00 43.73 ATOM 3767 CB LEU 494 71.692 8.000 2.366 1.00 43.38 ATOM 3770 CG LEU 494 71.692 8.000 2.366 1.00 43.38 ATOM 3771 CD LEU 494 71.563 0.614 2.431 1.00 42.55 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3778 CB ALA 495 75.466 0.838 4.551 1.00 43.80 ATOM 3778 CB ALA 495 75.668 0.838 4.551 1.00 48.52 ATOM 3778 CB ALA 495 75.668 0.838 4.551 1.00 48.52 ATOM 3788 CB GLU 496 77.330 1.258 3.104 1.00 49.79	CA GLY AGA	7.735 1 00 55 55
ATOM 3738 N GLN 491 67.073 13.304 5.634 1.00 54.79 ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 57.10 ATOM 3741 CB GLN 491 67.829 12.658 4.562 1.00 52.60 ATOM 3743 CD GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3744 OE1 GLN 491 70.046 13.666 1.00 57.19 ATOM 3745 NE2 GLN 491 70.046 13.669 1.548 1.00 62.09 ATOM 3745 NE2 GLN 491 70.046 13.669 1.548 1.00 62.09 ATOM 3748 C GLN 491 70.046 13.669 1.548 1.00 62.09 ATOM 3749 O GLN 491 69.669 11.704 5.605 1.00 49.56 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 49.56 ATOM 3751 CC VAL 492 68.705 9.093 5.456 1.00 49.56 ATOM 3755 CC VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3756 C VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 68.181 8.044 3.349 1.00 45.23 ATOM 3756 C VAL 492 68.181 8.044 3.349 1.00 45.23 ATOM 3760 CA VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3765 O VAL 493 71.608 7.478 2.706 1.00 45.23 ATOM 3760 CA VAL 493 71.608 7.478 2.706 1.00 44.71 ATOM 3760 CB VAL 493 71.608 7.478 2.706 1.00 42.06 ATOM 3767 CG LEU 494 71.682 3.158 3.142 1.00 42.06 ATOM 3767 CD LEU 494 71.682 3.158 3.142 1.00 42.06 ATOM 3768 CB LEU 494 71.682 3.158 3.142 1.00 42.06 ATOM 3777 CA ALA 495 76.059 4.032 3.821 1.00 43.38 ATOM 3777 CA ALA 495 76.059 4.032 3.103 1.00 43.78 ATOM 3778 CB ALA 495 76.059 4.032 3.103 1.00 43.78 ATOM 3779 C ALA 495 76.059 4.032 3.163 1.00 43.38 ATOM 3777 CA ALA 495 76.059 4.032 3.821 1.00 42.25 ATOM 3778 CB ALA 495 76.059 4.032 3.163 1.00 43.88 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 42.25 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.38 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.88 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.88 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3778 CB ALA 495 76.059 4.032 3.519 1.00 44.79 ATOM 3779 C ALA 495 76.059 4.032 3.519 1.00 48.52 ATOM 3778 CB ALA 495 76.059 4.032 3.519 1.00 48.52	7736 C GLY 490	7.143 1 00 55 60
ATOM 3740 CA GLN 491 67.073 13.304 5.664 1.00 57.10 ATOM 3741 CB GLN 491 67.829 12.658 4.562 1.00 57.10 ATOM 3742 CG GLN 491 68.760 13.580 3.777 1.00 53.44 ATOM 3743 CD GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3745 NE2 GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3748 NE2 GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3749 NE2 GLN 491 70.113 14.893 1.701 1.00 70.26 ATOM 3750 N VAL 491 68.632 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.703 10.318 4.984 1.00 47.83 ATOM 3751 CB VAL 492 68.705 9.093 5.456 1.00 49.89 ATOM 3755 CC2 VAL 492 67.760 8.320 6.412 1.00 46.38 ATOM 3755 CC2 VAL 492 67.361 9.211 7.606 1.00 46.70 ATOM 3756 C VAL 492 68.181 8.044 3.349 1.00 45.21 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 45.21 ATOM 3762 CG1 VAL 493 70.599 6.780 3.109 1.00 45.17 ATOM 3763 CG2 VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3765 C VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.75 ATOM 3767 C VAL 493 71.205 5.482 3.624 1.00 43.75 ATOM 3767 C VAL 493 71.508 8.902 1.838 1.00 46.16 ATOM 3768 C A LEU 494 71.608 7.471 2.148 1.00 43.38 ATOM 3768 C A LEU 494 71.608 1.158 3.142 1.00 43.38 ATOM 3767 C CD LEU 494 71.608 1.00 43.38 ATOM 3768 C A LEU 494 71.608 1.00 43.38 ATOM 3769 C B LEU 494 71.608 1.00 43.38 ATOM 3770 C C LEU 494 71.608 1.00 43.38 ATOM 3771 C A LLA 495 75.456 1.00 43.60 ATOM 3775 C A ALA 495 75.456 1.00 43.60 ATOM 3777 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3778 C B ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3779 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3779 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3778 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3778 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3778 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3737 () CLV	5.993 1 00 54 70
ATOM 3740 CA GLN 491 67.073 13.304 5.634 1.00 53.48 ATOM 3741 CB GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3743 CD GLN 491 68.760 13.580 3.777 1.00 53.48 ATOM 3744 OEI GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3748 C GLN 491 70.113 14.893 1.701 1.00 70.26 ATOM 3749 O GLN 491 68.632 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 49.56 ATOM 3752 CA VAL 492 68.705 9.093 5.456 1.00 49.56 ATOM 3755 CB VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 CG2 VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 68.181 8.044 3.349 1.00 45.61 ATOM 3757 O VAL 492 68.181 8.044 3.349 1.00 45.23 ATOM 3760 CA VAL 493 70.210 7.654 4.208 1.00 45.23 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3763 CG2 VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3763 CG2 VAL 493 71.159 8.902 1.838 1.00 46.16 ATOM 3766 C VAL 493 71.608 7.471 2.148 1.00 42.06 ATOM 3767 CG LEU 494 71.602 7.455 1.00 43.38 ATOM 3767 CG LEU 494 71.602 7.455 1.00 43.38 ATOM 3767 CG LEU 494 71.602 7.455 1.00 43.38 ATOM 3768 CA LEU 494 71.602 7.455 1.00 43.38 ATOM 3767 CG LEU 494 71.602 7.455 1.00 43.38 ATOM 3768 CA LEU 494 71.602 7.455 1.00 43.38 ATOM 3769 CB LEU 494 71.602 3.158 3.142 1.00 43.29 ATOM 3767 CG LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3767 CG LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3768 CB LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3769 CB LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3767 CG LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.83 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.83 ATOM 3778 C ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3778 CB ALA 495 76.059 4.032 3.519 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3738 N GIN	03.35/ 11.854 5 366
ATOM 3741 CB GLN 491 ATOM 3742 CG GLN 491 ATOM 3743 CD GLN 491 ATOM 3744 OEI GLN 491 ATOM 3744 OEI GLN 491 ATOM 3745 NE2 GLN 491 ATOM 3746 C GLN 491 ATOM 3749 O GLN 491 ATOM 3750 N VAL 492 ATOM 3752 CA VAL 492 ATOM 3754 CGI VAL 492 ATOM 3755 CG2 VAL 492 ATOM 3755 CG2 VAL 492 ATOM 3756 C VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 492 ATOM 3758 N VAL 492 ATOM 3756 C VAL 492 ATOM 3756 CA VAL 493 ATOM 3757 O VAL 492 ATOM 3756 C VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 492 ATOM 3758 N VAL 493 ATOM 3760 CA VAL 493 ATOM 3761 CB VAL 493 ATOM 3762 CGI VAL 493 ATOM 3763 CG2 VAL 493 ATOM 3764 C VAL 493 ATOM 3765 O VAL 493 ATOM 3766 C VAL 493 ATOM 3767 CA ALA 494 ATOM 3767 CG LEU 494 ATOM 3767 CG LEU 494 ATOM 3769 CB LEU 494 ATOM 3769 CB LEU 494 ATOM 3769 CB LEU 494 ATOM 3770 CG LEU 494 ATOM 3777 CA ALA 495 ATOM 3777 CA ALA 495 ATOM 3779 C ALA 495 ATOM 3788 N GLU 496 ATOM 3788 N GLU 496 ATOM 3788 O ALA 495 ATOM 3788 C B ALA 495 ATOM 3788 O ALA 495 ATOM 3788 C B ALA 495 ATOM 3788 O ALA 495 ATOM 3788 C B ALA 496 ATOM 3788 C B ALA 495 ATOM 3788 C B ALA 495 ATOM 3788 C B ALA 495 ATOM 3788 C B ALA 49	ATOM 3740 CA CLA	67.073 13.304 5 634
ATOM 3742 CG GLN 491 ATOM 3744 OE1 GLN 491 ATOM 3745 NE2 GLN 491 ATOM 3749 O GLN 491 ATOM 3750 N VAL ATOM 3753 CB VAL 492 ATOM 3755 CG2 VAL ATOM 3756 C VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 492 ATOM 3758 N VAL 493 ATOM 3756 C VAL 494 ATOM 3757 O VAL 494 ATOM 3758 N VAL 494 ATOM 3758 N VAL 495 ATOM 3758 N VAL 494 ATOM 3758 N VAL 495 ATOM 3758 N VAL 493 ATOM 3756 CA VAL 493 ATOM 3756 CA VAL 493 ATOM 3756 CB VAL 493 ATOM 3757 CA VAL 493 ATOM 3757 CG2 VAL 493 ATOM 3758 N VAL 493 ATOM 3759 CG2 VAL 493 ATOM 3750 CG2 VAL 493 ATOM 3751 CB VAL 493 ATOM 3750 CC2 VAL 493 ATOM 3750 CC3 VAL 493 ATOM 3750 CC4 VAL 493 ATOM 3750 CC6 VAL 493 ATOM 3750 CC7 VAL 493 ATOM 3750 CC7 VAL 493 ATOM 3750 CC8 VAL 493 ATOM 3750 CC9 VAL 493 ATOM 3760 CA VAL 493 ATOM 3760 CB VAL 494 ATOM 3760 CB VAL 494 ATOM 3760 CB VAL 494 ATOM 3760 CB VAL 495 ATOM 3770 CB VAL 494 ATOM 3770 CB VAL 494 ATOM 3770 CB VAL 495 ATOM 3770 CD VAL	ATOM 3741 CB CLN	67.829 12 550
ATOM 3744 CB GLN 491 ATOM 3745 NE2 GLN 491 ATOM 3746 NE2 GLN 491 ATOM 3748 C GLN 491 ATOM 3749 O GLN 491 ATOM 3750 N VAL 492 ATOM 3751 CB VAL 492 ATOM 3752 CA VAL 492 ATOM 3754 CGI VAL 492 ATOM 3755 CG VAL 492 ATOM 3756 C VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 492 ATOM 3756 C VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 493 ATOM 3756 C VAL 492 ATOM 3756 C VAL 492 ATOM 3757 O VAL 493 ATOM 3756 C VAL 492 ATOM 3757 O VAL 493 ATOM 3756 C VAL 493 ATOM 3757 O VAL 493 ATOM 3756 C VAL 493 ATOM 3757 O VAL 493 ATOM 3756 C VAL 493 ATOM 3757 O VAL 493 ATOM 3756 C VAL 493 ATOM 3757 O VAL 493 ATOM 3757 O VAL 493 ATOM 3756 C VAL 493 ATOM 3757 O VAL 493 ATOM 3756 C VAL 493 ATOM 3757 O VAL 493 ATOM 3756 C VAL 493 ATOM 3757 O VAL 493 ATOM 3757 O VAL 493 ATOM 3758 CB VAL 493 ATOM 3757 O VAL 493 ATOM 3757 O VAL 493 ATOM 3758 CB VAL 493 ATOM 3758 CB VAL 493 ATOM 3757 O VAL 493 ATOM 3757 O VAL 493 ATOM 3758 CB VAL 493 ATOM 3758 CB VAL 493 ATOM 3760 CA VAL 493 ATOM 3761 CB VAL 493 ATOM 3762 CGI VAL 493 ATOM 3763 CB VAL 493 ATOM 3764 C VAL 493 ATOM 3765 O VAL 493 ATOM 3766 O VAL 493 ATOM 3767 C VAL 493 ATOM 3768 CB ALEU 494 ATOM 3768 CB ALEU 494 ATOM 3769 CB LEU 494 ATOM 3770 CG LEU 494 ATOM 3777 CA ALA 495 ATOM 3779 C A ALA 495 ATOM 3780 O ALA 495 ATOM 3781 N GLU 496 ATOM 3783 CA GLU 496 ATOM 3783 CA GLU 496 ATOM 3783 CA GLU 496 ATOM 3784 CB GLU 496 ATOM 3783 CA GLU 496 ATOM 3781 N GLU 496 ATOM 3783 CA GLU 496 ATOM 3784 CB GLU 496 ATOM 3788 C	ATOM 3742 CC 775	68.760 12 500 1.00 52.60
ATOM 3744 OEI GLN 491 70.046 13.696 1.548 1.00 62.09 ATOM 3745 NE2 GLN 491 70.113 14.893 1.701 1.00 70.26 ATOM 3749 O GLN 491 68.632 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 49.56 ATOM 3752 7A VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3755 CG VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3757 O VAL 492 68.181 8.044 3.349 1.00 46.61 ATOM 3758 N VAL 492 68.181 8.044 3.349 1.00 45.61 ATOM 3760 CA VAL 493 70.210 7.654 4.208 1.00 45.17 ATOM 3761 CB VAL 493 70.210 7.654 4.208 1.00 45.17 ATOM 3763 CG1 VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3766 C VAL 493 71.608 7.471 2.148 1.00 42.06 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3760 CG LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3760 CG LEU 494 71.563 0.614 2.431 1.00 43.29 ATOM 3767 CG LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3779 C ALEU 494 71.563 0.614 2.431 1.00 43.38 ATOM 3777 CD LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CB ALA 495 76.050 -0.337 1.760 1.00 42.50 ATOM 3775 CB ALA 495 76.050 -0.337 1.760 1.00 42.50 ATOM 3777 CD LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3779 C ALA 495 76.050 4.032 3.821 1.00 43.83 ATOM 3777 CA ALA 495 76.050 4.032 3.821 1.00 43.88 ATOM 3778 CB ALA 495 76.050 4.032 3.821 1.00 43.88 ATOM 3779 C ALA 495 76.050 4.032 3.821 1.00 43.88 ATOM 3779 C ALA 495 76.050 4.032 3.821 1.00 43.88 ATOM 3779 C ALA 495 76.050 4.032 3.821 1.00 43.88 ATOM 3779 C ALA 495 76.050 4.032 3.821 1.00 43.88 ATOM 3788 O ALA 495 76.050 4.032 3.821 1.00 43.88 ATOM 3788 N GLU 496 77.330 1.256 8.362 1.00 46.68 ATOM 3788 N GLU 496 77.330 1.256 8.3104 1.00 49.79	ATOM 3743 CD 574	69,422 12 810 1.00 53.48
ATOM 3745 NE2 GLN 491 70.113 14.893 1.701 1.00 62.09 ATOM 3748 C GLN 491 70.453 13.082 0.441 1.00 62.78 ATOM 3749 O GLN 491 68.632 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 49.89 ATOM 3751 CB VAL 492 68.705 9.093 5.456 1.00 47.83 ATOM 3752 CA VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3755 CG2 VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 C VAL 492 68.181 9.211 7.666 1.00 46.70 ATOM 3757 O VAL 492 68.181 8.044 ATOM 3758 N VAL 493 70.210 7.654 4.281 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 45.17 ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3765 O VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 N LEU 494 71.682 3.158 3.104 1.00 43.73 ATOM 3766 N LEU 494 71.205 5.482 3.624 1.00 43.38 ATOM 3767 CB LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3767 CG LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3767 CG LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3770 CG LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3771 CD1 LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3773 C LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3777 CG LEU 494 71.682 3.158 3.142 1.00 39.77 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.88 ATOM 3779 CA ALA 495 76.059 4.032 3.821 1.00 43.88 ATOM 3779 CA ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3744 075	70.046 13.606 2.629 1.00 57.19
ATOM 3748 C GLN 491 70.453 13.082 0.441 1.00 70.26 ATOM 3749 O GLN 491 68.632 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.632 11.518 5.165 1.00 49.89 ATOM 3752 CA VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3755 CE VAL 492 67.760 8.320 6.412 1.00 46.38 ATOM 3755 CC2 VAL 492 67.361 9.211 7.666 1.00 46.70 ATOM 3755 CC2 VAL 492 68.103 10.318 4.984 1.00 47.83 ATOM 3755 CC2 VAL 492 67.361 9.211 7.666 1.00 46.70 ATOM 3755 C VAL 492 68.181 8.044 3.349 1.00 45.23 ATOM 3758 N VAL 493 70.599 6.780 3.109 1.00 45.17 ATOM 3760 CA VAL 493 70.599 6.780 3.109 1.00 45.17 ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 N LEU 494 71.102 4.488 2.809 1.00 43.73 ATOM 3766 N LEU 494 71.625 5.482 3.624 1.00 43.73 ATOM 3766 CA LEU 494 71.682 3.158 3.142 1.00 43.73 ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.29 ATOM 3771 CD1 LEU 494 71.689 0.201 3.850 1.00 39.77 ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 3.772 CD2 LEU 494 70.600 -0.337 1.760 3.772 CD2 LEU 494 71.689 0.201 3.850 1.00 43.83 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 42.702 ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.83 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.76 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.76 ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.256 3.190 1.00 49.79	7004	70.113 14 803 1.348 1.00 62.09
ATOM 3749 O GLN 491 68.632 11.518 5.165 1.00 49.89 ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 47.83 ATOM 3752 7A VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3753 CB VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 CG2 VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3757 O VAL 492 68.118 8.044 3.349 1.00 46.79 ATOM 3758 N VAL 492 68.181 8.044 3.349 1.00 45.23 ATOM 3756 C VAL 492 68.181 8.044 3.349 1.00 45.17 ATOM 3760 CA VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 N LEU 493 71.205 5.482 3.624 1.00 42.06 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3766 N LEU 494 71.602 5.482 3.158 3.142 1.00 43.29 ATOM 3769 CB LEU 494 70.988 2.030 2.366 1.00 43.29 ATOM 3770 CG LEU 494 70.600 -0.337 1.760 1.00 43.29 ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3772 CD LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3773 C LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 N ALA 495 75.456 2.785 3.183 1.00 42.06 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.83 ATOM 3779 C BEL 494 73.139 3.280 2.725 1.00 42.72 ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.83 ATOM 3779 C BALA 495 75.456 2.785 3.183 1.00 43.83 ATOM 3779 C BALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 76.6171 1.546 3.682 1.00 43.73 ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 76.671 1.546 3.682 1.00 43.76 ATOM 3780 O ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3740 0	70.453 13.000 1.701 1.00 70.26
ATOM 3750 N VAL 492 68.103 10.318 4.984 1.00 49.56 ATOM 3753 CB VAL 492 68.705 9.093 5.456 1.00 49.58 ATOM 3753 CB VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 C62 VAL 492 67.361 9.211 7.666 1.00 46.70 ATOM 3756 C VAL 492 67.361 9.211 7.666 1.00 46.97 ATOM 3757 O VAL 492 68.181 8.044 3.349 1.00 45.17 ATOM 3758 N VAL 493 70.599 6.780 31.09 40.471 ATOM 3761 CB VAL 493 70.599 6.780 31.09 1.00 44.71 ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3765 C VAL 493 71.159 8.902 1.838 1.00 46.16 ATOM 3766 N LEU 494 71.602 7.428 2.706 1.00 42.06 ATOM 3766 N LEU 494 71.602 3.624 1.00 43.73 ATOM 3766 CB LEU 494 71.602 3.158 3.142 1.00 43.38 ATOM 3767 CG LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3771 CD1 LEU 494 71.602 3.158 3.142 1.00 43.29 ATOM 3773 C LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3773 C LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3773 C LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3777 CG LEU 494 70.998 2.725 1.00 42.50 ATOM 3778 CB ALA 495 74.044 2.698 3.499 1.00 42.72 ATOM 3779 C A ALA 495 74.044 2.698 3.189 1.00 43.88 ATOM 3779 C A ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3779 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3779 C A ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3779 C A ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3780 O ALA 495 75.668 0.838 4.551 1.00 49.79	ATOM 3740 " GLN 491	68 632 11 0.441 1.00 62.78
ATOM 3752 CA VAL 492 68.103 10.318 4.984 1.00 47.83 ATOM 3753 CB VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 CG2 VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3756 C VAL 492 67.361 9.211 7.666 1.00 46.70 ATOM 3757 O VAL 492 69.004 8.200 4.253 1.00 45.23 ATOM 3758 N VAL 493 70.210 7.654 4.208 1.00 45.17 ATOM 3760 CA VAL 493 70.599 6.780 3.109 1.00 43.75 ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 N LEU 494 71.002 5.482 3.624 1.00 44.09 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3768 CA LEU 494 71.682 3.158 3.142 1.00 43.29 ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3773 C LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3773 C LEU 494 71.689 0.201 3.850 1.00 42.50 ATOM 3775 CA ALA 495 74.044 2.698 3.499 1.00 42.50 ATOM 3777 CA ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 377	69 660 1. 5.165 1.00 49.89
ATOM 3753 CB VAL 492 68.705 9.093 5.456 1.00 46.38 ATOM 3755 CG2 VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 CG2 VAL 492 67.361 9.211 7.606 1.00 46.70 ATOM 3757 0 VAL 492 69.004 8.200 4.253 1.00 45.23 ATOM 3758 N VAL 493 70.210 7.654 4.208 1.00 45.17 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 45.17 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.159 8.902 1.838 1.00 46.16 ATOM 3766 N LEU 494 71.602 4.448 2.809 1.00 43.78 ATOM 3768 CA LEU 494 71.602 4.448 2.809 1.00 43.78 ATOM 3769 CB LEU 494 71.662 3.158 3.162 1.00 43.38 ATOM 3771 CD1 LEU 494 71.662 3.158 3.162 1.00 43.38 ATOM 3772 CD2 LEU 494 71.662 3.158 3.158 3.142 1.00 3.38 ATOM 3773 C LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3776 CB LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3775 CD2 LEU 494 71.563 0.614 2.431 1.00 42.50 ATOM 3775 CA ALA 495 76.059 4.032 3.821 1.00 43.88 ATOM 3777 CA ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79 ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	N VAL 493	5.805 1 00 40 55
ATOM 3754 CB VAL 492 67.760 8.320 6.412 1.00 45.61 ATOM 3755 CG2 VAL 492 67.361 9.211 7.606 1.00 45.61 ATOM 3756 C VAL 492 69.004 8.200 4.253 1.00 45.23 ATOM 3761 CB VAL 493 70.210 7.654 4.208 1.00 45.17 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.159 8.902 1.838 1.00 46.20 ATOM 3766 N LEU 494 71.205 5.482 3.624 1.00 43.78 ATOM 3768 CA LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3770 CG LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3771 CD1 LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3772 CD2 LEU 494 71.600 -0.337 1.760 1.00 42.50 ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 42.50 ATOM 3777 CA ALA 495 76.059 4.032 3.821 1.00 42.50 ATOM 3777 CA ALA 495 76.059 4.032 3.821 1.00 42.50 ATOM 3777 CA ALA 494 71.563 0.614 2.431 1.00 39.77 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.83 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.83 ATOM 3779 C ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3779 C ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79 ATOM 3781 CB GLU 496 77.330 1.258 3.104 1.00 49.79 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79	A VAL 492	4.984 1 00 47 55
ATOM 3755 CG2 VAL 492 68 412 7.045 6.912 1.00 45.61 ATOM 3756 C VAL 492 69.004 8.200 4.253 1.00 45.23 ATOM 3758 N VAL 493 70.210 7.654 4.208 1.00 45.17 ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71 ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3763 CG2 VAL 493 71.608 7.471 2.148 1.00 46.20 ATOM 3766 N LEU 493 71.205 5.482 3.624 1.00 44.09 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.78 ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29 ATOM 3770 CG LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3771 CD1 LEU 494 71.600 -0.337 1.700 3772 CD2 LEU 494 71.600 -0.337 1.700 3773 C LEU 494 71.600 -0.337 1.700 3775 N ALA 495 74.044 2.698 3.499 1.00 42.50 ATOM 3777 CA ALA 495 74.044 2.698 3.499 1.00 42.50 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3777 CA ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 75.668 0.838 4.551 1.00 43.76 ATOM 3780 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79 ATOM 3781 CB GLU 496 77.330 1.258 3.104 1.00 49.79 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79	3753 CB VAL 492	5.456 1 00 46 30
ATOM 3755 CG2 VAL 492 67.361 9.211 7.6C6 1.00 46.97  ATOM 3757 O VAL 492 69.004 8.200 4.253 1.00 45.23  ATOM 3758 N VAL 493 70.210 7.654 4.208 1.00 45.17  ATOM 3760 CA VAL 493 70.599 6.780 3.109 1.00 43.75  ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 46.20  ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20  ATOM 3764 C VAL 493 71.59 8.902 1.838 1.00 46.16  ATOM 3765 O VAL 493 71.205 5.482 2.706 1.00 42.06  ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73  ATOM 3768 CA LEU 494 71.102 4.448 2.809 1.00 43.38  ATOM 3769 CB LEU 494 70.988 2.030 2.366 1.00 43.38  ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38  ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77  ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 42.50  ATOM 3773 C LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3777 CA ALA 495 74.044 2.698 3.499 1.00 43.83  ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.80  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 43.76  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 43.76  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	3754 CG1 VAL 492	6.412 1 00 45 61
ATOM 3756 C VAL 492 69.004 8.200 4.253 1.00 45.23   ATOM 3757 O VAL 492 68.181 8.044 3.349 1.00 45.17   ATOM 3760 CA VAL 493 70.210 7.654 4.208 1.00 43.75   ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71   ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20   ATOM 3763 CG2 VAL 493 71.159 8.902 1.838 1.00 46.16   ATOM 3765 O VAL 493 71.205 5.482 3.624 1.00 44.09   ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73   ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.38   ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29   ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38   ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77   ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 42.50   ATOM 3773 C LEU 494 73.139 3.280 2.725 1.00 42.72   ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.83   ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80   ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76   ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79   ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79   ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	A10M 3755 CG2 TAT	7.045 6.932 1.00 46 70
ATOM 3758 N VAL 493 70.210 7.654 4.208 1.00 45.17  ATOM 3760 CA VAL 493 70.210 7.654 4.208 1.00 43.75  ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 44.71  ATOM 3763 CG2 VAL 493 71.159 8.902 1.838 1.00 44.71  ATOM 3765 C VAL 493 71.205 5.482 3.624 1.00 46.16  ATOM 3766 N LEU 494 71.701 5.402 4.745 1.00 43.73  ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.38  ATOM 3770 CG LEU 494 71.809 0.201 3.850 1.00 43.38  ATOM 3771 CD1 LEU 494 71.809 0.201 3.850 1.00 36.38  ATOM 3773 C LEU 494 71.809 0.201 3.850 1.00 36.38  ATOM 3774 C LEU 494 73.435 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.80  ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3756 C VAL. 400	9.211 7.605
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ATOM 3760 CA VAL 493 70.599 6.780 3.109 1.00 43.75  ATOM 3761 CB VAL 493 70.599 6.780 3.109 1.00 44.71  ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 46.20  ATOM 3763 CG2 VAL 493 71.159 8.902 1.838 1.00 46.16  ATOM 3764 C VAL 493 71.205 5.482 3.624 1.00 42.06  ATOM 3765 O VAL 493 71.701 5.402 4.745 1.00 43.73  ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.38  ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29  ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38  ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77  ATOM 3772 CD2 LEU 494 71.809 0.201 3.850 1.00 36.38  ATOM 3773 C LEU 494 70.600 -0.337 1.760 1.00 42.50  ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.83  ATOM 3777 CA ALA 495 74.044 2.698 3.499 1.00 43.80  ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.76  ATOM 3780 O ALA 495 75.668 0.838 4.551 1.00 43.76  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3758 N VAT	68.181 8.044 3.240 1.50 45.23
ATOM 3761 CB VAL 493 71.608 7.471 2.148 1.00 44.71 ATOM 3762 CG1 VAL 493 71.159 8.902 1.838 1.00 46.16 ATOM 3763 CG2 VAL 493 73.045 7.428 2.706 1.00 42.06 ATOM 3765 O VAL 493 71.205 5.482 3.624 1.00 44.09 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3768 CA LEU 494 71.682 3.158 3.142 1.00 43.29 ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3771 CD1 LEU 494 71.809 0.201 3.850 1.00 39.77 ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 42.50 ATOM 3773 C LEU 494 73.139 3.280 2.725 1.00 42.72 ATOM 3774 O LEU 494 73.435 3.929 1.720 1.00 43.83 ATOM 3777 CA ALA 495 74.044 2.698 3.499 1.00 43.83 ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3760 CA VAL	70.210 7.654 4 309 1 3
ATOM 3762 CG1 VAL 493 71.608 7.471 2.148 1.00 44.71  ATOM 3763 CG2 VAL 493 73.045 7.428 2.706 1.00 46.16  ATOM 3764 C VAL 493 71.205 5.482 3.624 1.00 44.09  ATOM 3766 N LEU 494 71.701 5.402 4.745 1.00 43.73  ATOM 3768 CA LEU 494 71.682 3.158 3.142 1.00 43.38  ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29  ATOM 3770 CG LEU 494 71.563 0.614 2.431 1.00 39.77  ATOM 3771 CD1 LEU 494 71.809 0.201 3.850 1.00 36.38  ATOM 3773 C LEU 494 70.600 -0.337 1.760 1.00 42.50  ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3777 CA ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3779 C ALA 495 75.456 2.785 3.183 1.00 43.80  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 O ALA 495 75.668 0.838 4.551 1.00 43.76  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3783 CA GLU 496 78.112 0.103 3.519 1.00 49.79	ATOM 3761 CB VAL	70.599 6.780 3 100 1.00 43.75
ATOM 3763 CG2 VAL 493 71.159 8.902 1.838 1.00 46.20 ATOM 3764 C VAL 493 73.045 7.428 2.706 1.00 42.06 ATOM 3765 O VAL 493 71.205 5.482 3.624 1.00 44.09 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3768 CA LEU 494 71.682 3.158 3.142 1.00 43.38 ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3771 CD1 LEU 494 71.809 0.201 3.850 1.00 43.38 ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 39.77 ATOM 3773 C LEU 494 70.600 -0.337 1.760 1.00 36.38 ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.50 ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.83 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3780 O ALA 495 76.568 0.838 4.551 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3762 CC1 VIII	71.608 7.421
ATOM 3764 C VAL 493 73.045 7.428 2.706 1.00 42.06 ATOM 3765 O VAL 493 71.205 5.482 3.624 1.00 44.09 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29 ATOM 3770 CG LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3771 CD1 LEU 494 71.809 0.201 3.850 1.00 36.38 ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 42.50 ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72 ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.80 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 43.76 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3783 CA GLU 496 78.112 0.103 3.519 1.00 49.79	ATOM 3763	71.159 9.000 2.148 1.00 46.20
ATOM 3765 O VAL 493 71.205 5.482 3.624 1.00 42.06 ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29 ATOM 3770 CG LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3771 CD1 LEU 494 71.809 0.201 3.850 1.00 36.38 ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 42.50 ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72 ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.83 ATOM 3777 CA ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 48.52 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.79	ATOM 3764 C 493	73.045 7.420 1.038 1.00 46.16
ATOM 3766 N LEU 494 71.102 4.448 2.809 1.00 43.73 ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29 ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38 ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77 ATOM 3772 CD2 LEU 494 71.809 0.201 3.850 1.00 36.38 ATOM 3773 C LEU 494 70.600 -0.337 1.760 1.00 42.50 ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72 ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.83 ATOM 3777 CA ALA 495 74.044 2.698 3.499 1.00 40.80 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3783 CA GLU 496 78.524 -0.733	ATOM 375	71.205 5.402 2.706 1.00 42.06
ATOM 3768 CA LEU 494 71.102 4.448 2.809 1.00 43.73  ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29  ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38  ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77  ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 36.38  ATOM 3773 C LEU 494 73.139 3.280 2.725 1.00 42.50  ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.83  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3783 CA GLU 496 78.524 70.722	ATOM 3766 W	71.701 5.024 1.00 44.09
ATOM 3769 CB LEU 494 71.682 3.158 3.142 1.00 43.29  ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.38  ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77  ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 36.38  ATOM 3773 C LEU 494 73.139 3.280 2.725 1.00 42.50  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 C ALA 495 75.668 0.838 4.551 1.00 48.52  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3783 CA GLU 496 78.524 70.725	ATOM 3768 - LEU 494	71.102 4.442 4.743 1.00 43.73
ATOM 3770 CG LEU 494 70.988 2.030 2.366 1.00 43.29  ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77  ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 36.38  ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.50  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.83  ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 O ALA 495 75.668 0.838 4.551 1.00 48.52  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3784 CB GLU 496 78.524 70.725	ATOM 3760 THEU 494	71 602 2.809 1.00 43.38
ATOM 3771 CD1 LEU 494 71.563 0.614 2.431 1.00 39.77  ATOM 3772 CD2 LEU 494 70.600 -0.337 1.760 1.00 42.50  ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.80  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 O ALA 495 75.668 0.838 4.551 1.00 48.52  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3784 CB GLU 496 78.524 70.722	ATOM 3703 CB LEU 494	70 000 3.142 1.00 43 29
ATOM 3772 CD2 LEU 494 71.809 0.201 3.850 1.00 36.38  ATOM 3773 C LEU 494 70.600 -0.337 1.760 1.00 42.50  ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.83  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.80  ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3783 CA GLU 496 78.524 70.726	ATOM LEU 494	71 563 2.030 2.366 1.00 43 38
ATOM 3773 C LEU 494 70.600 -0.337 1.760 1.00 36.38  ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.80  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3784 CB GLU 496 78.524 70.726	3771 CD1 LEU 494	71 700 2.431 1.00 39 77
ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.80  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68  ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3783 CA GLU 496 78.112 0.103 3.519 1.00 49.79	3/72 CD2 LEU 494	3.850 1.00 36 30
ATOM 3774 O LEU 494 73.139 3.280 2.725 1.00 42.72  ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 40.80  ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.80  ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76  ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68  ATOM 3781 N GLU 496 75.668 0.838 4.551 1.00 48.52  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3784 CB GLU 496 78.524 70.733	ATOM 3773 C LEU 494	70.600 -0.337 1.760 1 00 43 50
ATOM 3775 N ALA 495 74.044 2.698 3.499 1.00 43.83 ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68 ATOM 3781 N GLU 496 75.668 0.838 4.551 1.00 48.52 ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3784 CB GLU 496 78.524 70.733	ATOM 3774 O LEU 494	73.139 3.280 2.725 1 00 42 72
ATOM 3777 CA ALA 495 75.456 2.785 3.183 1.00 40.80 ATOM 3778 CB ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 43.76 ATOM 3781 N GLU 496 75.668 0.838 4.551 1.00 48.52 ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3784 CB GLU 496 78.524 70.733	ATOM 3775 N ATA 100	73.435 3.929 1 720
ATOM 3778 CB ALA 495 75.456 2.785 3.183 1.00 43.80 ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68 ATOM 3781 N GLU 496 75.668 0.838 4.551 1.00 48.52 ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3784 CB GLU 496 78.524 70.733	ATOM 3777 CA ATA 405	74.044 2.698 3.499 1.50 43.83
ATOM 3779 C ALA 495 76.059 4.032 3.821 1.00 43.76 ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 46.68 ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3784 CB GLU 496 78.524 70.733	ATOM 3778 CB NIN	75.456 2.785 3.182 1.00 40.80
ATOM 3780 O ALA 495 76.171 1.546 3.682 1.00 43.76  ATOM 3781 N GLU 496 75.668 0.838 4.551 1.00 48.52  ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13  ATOM 3784 CB GLU 496 78.112 0.103 3.519 1.00 49.79	ATOM 3779 C 333	76.059 4.032 3 821 1 22
ATOM 3781 N GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3784 CB GLU 496 78.524 70.733 3.519 1.00 49.79	ATOM 3780 0 378	76.171 1 546 3.021 1.00 43.76
ATOM 3783 CA GLU 496 77.330 1.258 3.104 1.00 49.13 ATOM 3784 CB GLU 496 78.112 0.103 3.519 1.00 49.79	ATOM 3701 W ALA 495	75.668 0.000 3.662 1.00 46.68
ATOM 3784 CB GLU 496 78.112 0.103 3.519 1.00 49.13	ATOM 3783 CT 496	77.330 1.350 1.00 48.52
78.524 TO 33.519 1.00 49.79	ATOM 3704 CA GLU 496	78.112 0 103 3.104 1.00 49.13
2.318 1.00 53.83	3/64 CB GLU 496	78.524 =0.730 3.519 1.00 49.79
		2.318 1.00 53.83

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1.496 ATOM 3785 CG GLU 496 77.350 -1.224 1.00 61.33 ATOM 3786 CD GLU 496 77.623 -2.561 0.862 1.00 64.74 ATOM 3787 OE1 GLU 496 76.704 0.883 -3.411 1.00 70.08 ATOM 3788 OE2 GLU 496 78.751 -2.760 0.356 1.00 64.12 ATOM 3789 С GLU 496 79.333 0.601 4.230 1.00 48.46 MOTA 3790 0 GLU 496 80.192 1.236 1.00 48.79 3.631 **ATOM** 3791 N ALA 497 79.373 0.375 5.530 1.00 49.25 **ATOM** 3793 CA ALA 497 80.503 0.810 6.334 1.00 49.99 **ATOM** 3794 CB ALA 497 80.048 1.156 7.732 1.00 48.16 ATOM 3795 С ALA 497 81.544 -0.301 6.373 1,00 51.53 ATOM 3796 0 ALA 497 -1.473 81.191 6.409 1.00 52.41 ATOM 3797 N ILE 498 82.821 0.061 6.335 1.00 52.35 3799 ATOM CA ILE 498 83.892 -0.928 6.369 1.00 52.03 **ATOM** 3800 CB ILE 498 84.843 -0.797 5.145 1.00 52.83 ATOM 3801 CG2 ILE 498 85.990 -1.795 5.253 1.00 51.43 ATOM 3802 CG1 ILE 498 84.077 -1.006 3.830 1.00 53.85 **ATOM** 3803 CD1 ILE 498 83.411 0.254 3.271 1.00 55.62 ATOM 3804 C ILE 498 84.702 -0.802 7.654 1.00 52.74 **ATOM** 3805 0 ILE 498 85.133 0.293 8.026 1.00 52.14 ATOM 3806 N GLY 499 84.835 -1.926 8.354 1.00 52.58 ATOM 3808 CA GLY 499 85.600 -1.974 9.592 1.00 53.03 **ATOM** 3809 Ċ. GLY 499 10.771 85.165 -1.113 1.00 53.67 . ATOM 3810 O GLY 499 86.012 -0.544 11.463 1.00 53.99 ATOM 3811 N LEU 500 83.862 -1.045 11.034 1.00 53.60 MOTA 3813 CA LEU 500 83.337 -0.245 12.141 1.00 51.00 MOTA 3814 CB LEU 500 81.841 -0.499 12.317 1.00 49 38 MOTA. 3815 CG LEU 500 80.901 -0.024 11.212 1.00 47.62 MOTA CD1 LEU 3816 500 79.483 -0.454 11.543 1.00 47.25 MOTA CD2 LEU 3817 500 80.992 1.486 11.081 1.00 47.38 ATOM 3818 C LEU 500 84.060 -0.573 13.433 1.00 51.05 **ATOM** 3819 0 LEU 500 84.396 -1.734 13.670 1.00 53.76 MOTA . 3820 N PRO 87.588 505 -5.968 10.545 1.00 81.81 **ATOM** 3821 CD PRO 505 88.588 ~6.677 11.357 1.00 81.96 **ATOM** 3822 CA PRO 10.109 505 88.105 -4.664 1.00 80.56 **ATOM** 3823 CB PRO 505 89.501 -4.622 10.735 1.00 80.75 ATOM 3824 CG PRO 505 89.868 -6.070 10.860 1.00 82.32 **ATOM** 3825 С PRO 1.00 78.53 505 88.139 -4.477 8.588 **ATOM** 3826 0 PRO 505 88.462 -3.400 8.085 1.00 77.85 MOTA 3827 N ASN 506 87.792 -5.532 7.865 1.00 77.09 MOTA 3829 CA ASN 506 87.747 -5.484 6.411 1.00 75.57 ATOM 3830 88.799 CB ASN 506 -6.415 5.806 1.00 75.80 **ATOM** 3831 C ASN 506 86.347 -5.929 6.008 1.00 74.33 ATOM 3832 0 ASN 506 86.044 -6.117 4.826 1.00 73.76 **ATOM** 3833 N ARG 507 85.496 -6.092 7.018 1.00 71.72 ATOM 3835 CA ARG 507 84.120 -6.509 6.820 1.00 69.28 ATOM 3836 CB ARG 507 83.619 -7.257 8.054 1.00 70.64 MOTA 3837 С ARG 507 83.258 -5.284 6.605 1.00 65.87 MOTA 3838 О ARG 507 83.445 -4.262 7.274 1.00 65.40 MOTA 3839 N VAL 508 82.363 -5.358 5.628 1.00 62.01 **ATOM** 3841 CA VAL 508 -4.248 81.464 5.381 1.00 58.41 MOTA 3842 CB VAL 508 81.043 -4.136 3.915 1.00 57.18 ATOM 3843 CG1 VAL 508 82.251 -3.893 3.046 1.00 61.04

	TOM 3844	CG2 1	VAL 508				
	FOM 3845		/AL 508	80.			6 1.00 60.74
ΓA	TOM 3846		/AL 508	80.2	- • •		6 1.00 56.61
AT	OM 3847		HR 509	79.9		716 6.52	
	OM 3849	_		79.5		6.66	
AT	OM 3850			78.3		7.50	
AT				78.7		44 8.93	
AT				79.9	38 -3.7		
AT	OM 3854	_		77.6	06 -3.5		
ATO				77.3	81 -2.6		
ATO	DM 3856			77.6	75 -1.5		1
ATO				76.23	38 -3.2		-0.55
ATC				75.20	02 -2.3		+ . / J
ATO				74.06			
ATO		CG LY		73.22			10.34
ATO		CD LY		73.82		•	1.00 54.93
ATO		CE LY		73.11			1.00 58.33
ATO		NZ LY		73.31			1.00 59.17
OTA		C LY		74.73		_	1.00 56.09
ATO	_	O LY	S 510	74.48		_	1.00 40.83
ATO		IAV N	<sup>լ</sup> . 511	74.67			1.00 38.59
ATOM		CA VAI		74.26			1.00 36.28
ATOM		CB VAI	511	75.480	–		1.00 31.41
		CG1 VAL	511	76.315		_	1.00 32.80
ATOM	7 7 7	CG2 VAI	511	76.353		•	1.00 29.97
ATOM	-5.5	C VAL	511	73.408	_		1.00 30.20
ATOM	- '	O VAL	511	73.305			1.00 28.40
ATOM		N ALA	512	72.756			1.00 27 45
ATOM	-0,5	CA ALA		71.953			1.00 27.30
ATOM	3880 (	B ALA	512	70.557			1.00 26.66
ATOM	3881 (	: ALA	512		3.640	8.278	1.00 24.24
ATOM	3882 (	ALA	512	72.670	4.965	8.173	1.00 28.52
ATOM	3883 N	VAL	513	73.140	5.036	9.319	1.00 26.66
ATOM	3885 C	A VAL	513	72.768	5.949	7.275	1.00 29.18
ATOM	3886 C	B VAL	513	73.442	7.217	7.569	1.00 29.65
ATOM		G1 VAL	513	74.631	7.482	6.601	1.00 28.93
ATOM	3888 C	G2 VAL	513	75.384	8.722	7.015	1.00 25.51
ATOM	3889 C		513	75.570	6.292	6.550	1.00 29.45
ATOM	3890 O	VAL	513	72.509	8.407	7.476	1.00 30.45
ATOM	3891 N	LYS	514	71.900	8.646	6.431	1.00 30.15
ATOM	3893 CZ		514	72.402	9.143	8.578 1	1.00 33.29
ATOM	3894 CE		514	71.575	10.357	8.654 1	.00 33.28
ATOM	3895 CG		514	71.017	10.537		.00 38.67
ATOM	3896 CD		514	70.074	9.456		.00 45.73
ATOM	3897 CE	_		69.462	9.860		.00 53.93
ATOM	3898 NZ		514	68.450	8.840		.00 63.59
MOTA	3902 C	LYS	514	67.206	8.823		.00 71.90
ATOM	3903 O		514	72.451	11.568		.00 29.45
ATOM	3904 N	LYS	514	73.584	11.673		.00 29,45
ATOM	3906 CA	MET	515	71.918	12.495		.00 25.64
ATOM	3907 CB	MET	515	72.668	13.690		00 29.42
ATOM	3908 CG	MET	515	73.464	13.391		00 30.46
ATOM	3909 SD	MET	515	72.557	13.070		00 29.63
	-303 SD	MET	515		12.475		00 32.48
						220 1.	00 33.06

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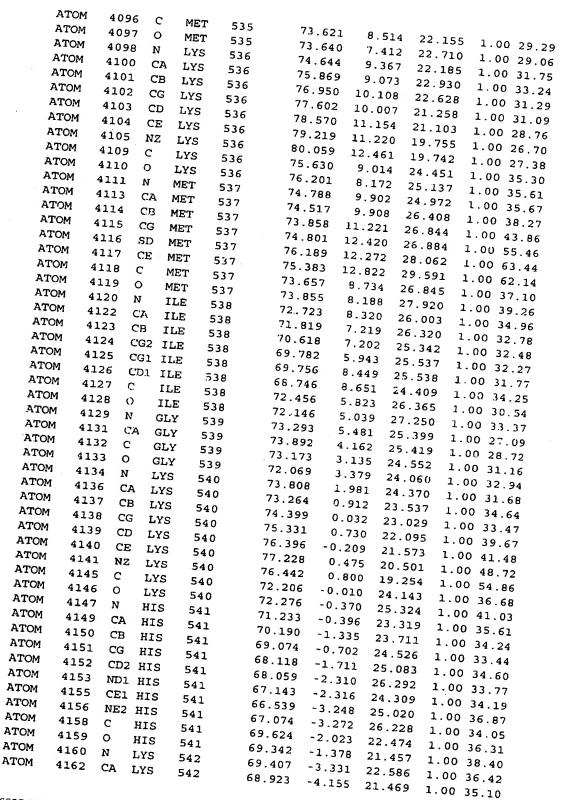
ATOM	3910	CE	MET	515	73.734	10.809	3.715	1.00 30.26
MOTA	3911	С	MET		71.700	14.839	6.848	1.00 30.75
ATOM	3912	0	MET	515	70.478	14.654	6.867	1.00 33.07
ATOM	3913	N	LEU		72.238	16.027	6.608	1.00 30.32
ATOM	3915	CA	LEU	516	71.414	17.194	6.304	1.00 30.21
MOTA	3916	CB	LEU		72.112	18.487	6.748	1.00 26.54
ATOM	3917	CG	LEU		72.452	18.668	8.227	1.00 23.97
ATOM	3918		LEU	516	73.345	19.858	8.412	1.00 24.27
ATOM	3919	CD2		516	71.198	18.850	9.023	1.00 21.46
ATOM	3920	С	LEU	516	71.197	17.265	4.800	1.00 33.44
MOTA	3921	0	LEU	516	72.016	16.784	4.015	1.00 34.50
ATOM	3922	N	LYS	517	70.082	17.863	4.400	1.00 36.36
MOTA	3924	CA	LYS	517	69.783	18.048	2.993	1.00 34.58
MOTA	3925	CB	LYS	517	68.281	18.255	2.784	1.00 38.96
ATOM	3926	CG	LYS	517	67.409	17.155	3.380	1.00 44.34
ATOM	3927	CD	LYS	517	66.128	16.920	2.572	1.00 52.11
ATOM	3928	CE	LYS	517	65.138	18.083	2.637	1.00 58.29
ATOM	3929	NZ	LYS	517	63.915	17.833	1.786	1.00 60.90
MOTA	3933	C	LYS	517	70.567	19.304	2.597	1.00 33.51
ATOM	3934	0	LYS	517	71.024	20.064	3.460	1.00 30.34
ATOM	3935	N	SER	518	70.701	19.539	1.296	1.00 34.39
ATOM	3937	CA	SER	518	71.444	20.693	0.788	1.00 35.84
ATOM	3938	CB	SER	518	71.537	20.618	-0.731	1.00 33.66
ATOM	3939	OG	SER	518	70.282	20.258	-1.266	1.00 38.73
ATOM	3941	C	SER	518	70.879	22.045	1.198	1.00 36.91
ATOM ATOM	3942	O N	SER	518	71.591	23.050	1.205	1.00 37.32
ATOM	3943	N	ASP ASP	519	69.598	22.069	1.538	1.00 37.88
ATOM	3945 3946	CA CB	ASP	519 519	68.945	23.313	1.936	1.00 38.63
ATOM	3947	CG	ASP	519	67.517	23.364	1.375	1 00 42.23
ATOM	3948		ASP	519	. 66.669 67.070	22.151 21.380	1.775 2.681	1.00 48.87 1.00 49.21
ATOM	3949		ASP	519	65.582	21.380	1.181	1.00 49.21
ATOM	3950	C	ASP	519	68.916	23.537	3.443	1.00 34.93
ATOM	3951	o	ASP	519	68.246	24.451	3.916	1.00 39.38
ATOM	3952	N	ALA	520	69.622	22.692	4.191	1.00 35.38
ATOM	3954	CA	ALA	520	69.631	22.795	5.648	1.00 34.69
ATOM	3955	СВ	ALA	520	70.359	21.613	6.259	1.00 35.68
ATOM	3956	C	ALA	520	70.213	24.087	6.173	1.00 33.54
ATOM	3957	0	ALA	520	71.039	24.718	5.522	1.00 34.83
ATOM	3958	N	THR	521	69.815	24.452	7.384	1.00 34.45
MOTA	3960	CA	THR	521	70.315	25.668	8.001	1.00 36.51
ATOM	3961	CB	THR	521	69.148	26.592	8.493	1.00 39.14
ATOM	3962	OG1	THR	521	68.529	26.031	9.659	1.00 41.61
MOTA	3964		THR	521	68.081	26.750	7.409	1.00 40.14
ATOM	3965	C	THR	521	71.228	25.303	9.170	1.00 36.35
ATOM	3966	0	THR	521	71.376	24.125	9.510	1.00 32.23
ATOM	3967	N	GLU	522	71.868	26.310	9.756	1.00 39.33
ATOM	3969	CA	GLU	522	72.747	26.092	10.890	1.00 44.59
ATOM	3970	CB	GLU	522	73.364	27.424	11.335	1.00 51.80
ATOM	3971	CG	GLU	522	74.463	27.311	12.418	1.00 64.10
ATOM	3972	CD	GLU	522	75.811	26.815	11.886	1.00 69.12
ATOM	3973	OE1	GLU	522	76.784	27.605	11.869	1.00 69.26

Δ	TOM	3054				
		3974	OE2	GLU	522	75.900 25.629 11 502
		3975	С	GLU :	522	71 053 11.302 1.00 73.62
	TOM :	3976	0	~	522	23.44/ 12.042 1.00 44 52
		3977			523	24.61/ 12.786 1 00 44 05
		979			523	70.679 25.814 12.167 1.00 42.00
A	rom 3	980				69.826 25.264 13 216 3 22
Α٦		981		••-	23	08.519 26.053 13 329 1 20
AT		982		•	23	67.583 25 502 2.00 45.99
АT		983	_		23	66.296 35 037 1.00 48.74
		984			23	65,405, 34, 303
AT					23	64.309 22 506 4 1.00 60.31
AT		988	_		23	69.563 22 702 47.247 1.00 65.17
ATO		989		YS 5	23	69 501 25.793 12.935 1.00 39.03
		90	N A	SP 52	24	69 333 34 13.850 1.00 40.65
ATO		92	C'A AS			23 43/ 11.672 1 00 34 03
ATO		93	CB AS			11.294 1 00 33 13
ATO		94	CG AS			08.876 21.942 9 790
ATC		95	OD1 AS			67.482 22.352 5 300 7 3
ATO	M 3.9		OD2 AS			66.552 22.193 70 204 1 00
ATO			-	_		67.307 33.036
ATO:			-	_		70.383 21 204 1.00 38.19
ATO			O AS		4	70.301 20.154
ATO			A LE		5	71.554 21.000 1-129 1.00 37.40
ATON		`	CA LEI		5	72 700
ATON		`	B LE	J 525	5	74 070 11.729 1.00 31.50
		_	'G LEU		;	75 363 11.278 1.00 29.05
ATOM			D1 LEC	J 525		11.680 1.00 20 20
ATOM			D2 LEU	_		13.390 11.065 1 00 27 27
ATOM		ნ ე	LEU			76.519 32.283 11.295 1 00 26 26
ATOM		7 0				72.848 30.941 13.221 1.00
ATOM		8 N				73.104 19.828 13 575
MOTA	4010					72.563 21.982 14 000 1 75
ATOM	4011			526		72.544 21.914 15.459 1.00 29.63
ATOM	4012			526		72.046 22.25
ATOM	4014			526		71, 923 22 100 = 1.00 32.03
ATOM	4015		SER	526		71.640 20 705
ATOM			SER	526		71.924 20 162 25.360 1.00 29.72
ATOM	4016		ASP	527		70.525 20.500
ATOM	4018			527		60 500
	4019	CB	ASP	527		69 222 13.356 15.664 1.00 29.28
ATOM	4020	CG	ASP	527		13./10 14.855 1 00 20 00
ATOM	4021	OD	1 ASP	527		15.225 1 00 30 05
ATOM	4022	OD:	2 ASP	527		21.39/ 16.292 1 00 24 32
ATOM	4023	C	ASP	527		00.591 21.335 14 436 1 22
ATOM	4024	0	ASP	527		70.175 18.164 15 426
ATOM	4025	N	LEU			70.115 17.297 16 313
ATOM	4027	CA		528		70.769 17.958 14 265 1 22 3
ATOM	4028	CB	LEU	528		71 350 16 665
ATOM	4029		LEU	528		71 850 16 645
ATOM		CG	LEU	528		72.409 15 330
ATOM	4030	CD1	LEU	528		71.466 74.742 1.00 24.26
	4031		LEU	528		73 644 12.259 1.00 21.51
ATOM	4032	C	LEU	528		72 404 10.450 1.00 15.05
ATOM	4033	0	LEU	528		10.342 14.933 1 00 30 53
ATOM	4034	N	ILE	529		72.641 15.192 15.354 1 00 30 70
ATOM	4036	CA	ILE	529		73.281 17.351 15.305 1 00 30 06
			_ <b>_</b>	-29		74.367 17.138 16.253 1.00 30.86
CCCD !=						2.00 28.41

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MOTA	4037	CB	ILE	529	75.266	18.349	16.406	1.00 24.75	
MOTA	4038	CG2	ILE	529	76.355	18.064	17.432	1.00 25.51	
MOTA	4039	CG1	ILE	529	75.901	18.710	15.084	1.00 17.82	
ATOM	4040	CD1	ILE	529	76.912	19.806	15.251	1.00 18.14	
ATOM	4041	С	ILE	529	73.821	16.813	17.641	1.00 30.17	
ATOM	4042	0	ILE	529	74.286	15.873	18.285	1.00 30.11	
MOTA	4043	N	SER	530	72.836	17.574	18.101	1.00 30.29	
ATOM	4045	CA	SER	530	72.271	17.310	19.418	1.00 33.14	
ATOM	4046	СВ	SER	530	71.158	18.293	19.735	1.00 36.09	
MOTA	4047	OG	SER	530	70.224	18.323	18.670	1.00 49.01	
ATOM	4049	C.	SER	530	71.740	15.881	19.479	1.00 33.80	
ATOM	4050	Ó	SER	530	71.896	15.190	20.492	1.00 37.06	
ATOM	4051	N	GLU	531	71.156	15.413	18.378	1.00 30.13	
MOTA	4053	CA	GLU	531	70.629	14.065	18.351	1.00 29.18	
ATOM	4054	CB	GLU	531	69.822	13.801	17.087	1.00 32.42	
ATOM	4055	CG	GLU	531	69.253	12.394	17.058	1.00 33.35	
ATOM	4056	CD	GLU	531	68:354	12.131	15.883	1.00 34.76	
ATOM	4057	OE1	GLU	531	67.481	11.249	16.002	1.00 40.42	
ATOM	4058	OE2	GLU	531	68.516	12:793	14.847	1.00 35.88	
ATOM	4059	C	GLU	531	71.734	13.025	18.488	1.00 28.27	
ATOM	4060	0	GLU	531	71.569	12.032	19.192	1.00 26.75	
ATOM	4061	N	MET	532	72.842	13.235	17.786	1.00 27.80	
ATOM	4063	CA	MET	532	73.976	12.320	17.835	1.00 27.82	
MOTA	4064	CB	MET	532	75.080	12.813	16.890	1.00 29.43	
MOTA	4065	CG	MET	532 .	76.461	1.2.225	17.138	1.00 24.34	
ATOM	4066	SD	MET	532	77.641	12.702	15.840	1.00 27.83	1
ATOM	4067	CE	MET	532	77.791.	14.452	16.193	1.00 21.90	
ATOM	4068	С	MET	532	74.499	12.272	19.260	1.00 29.53	
ATOM	4069	0	MET	532	74.742	11.197	19.809	1.00 30.14	
ATOM	4070	N	GLU	533	74.610	13.445	19.871	1.00 30.25	
ATOM	4072	CA	GLU	533	75.109	13.570	21.233	1.00 31.95	
ATOM	4073	CB	GLU	533	75.300	15.039	21.594	1.00 32.55	
ATOM	4074	CG	GLU	533	76.391	15.724	20.765	1.00 35.71	
ATOM	4075	CD	GLU	533	77.766	15.087	20.951	1.00 36.71	
ATOM	4076		GLU	533	78.297	15.136	22.084	1.00 40.19	
MOTA	4077	OE2	GLU	533	78.322	14.555	19.969	1.00 33.99	
ATOM	4078	C	GLU	533	74.185	12.886	22.225	1.00 33.06	
MOTA	4079	0	GLU	533	74.642	12.197	23.147	1.00 33.49	
MOTA	4080	N	MET	534	72.883	13.052	22.025	1.00 33.12	
ATOM	4082	CA	MET	534	71.913	12.432	22.900	1.00 32.48	
ATOM	4083	CB	MET	534	70.484	12.859	22.533	1.00 30.60	
ATOM	4084	CG	MET	534	69.591	12.915	23.791	0.50 28.70	PRT1
ATOM	4085	SD	MET	534	67.787	12.849	23.608	0.50 27.55	PRT1
ATOM	4086	CE	MET	534	67.409	14.560	23.291	0.50 26.84	PRT1
ATOM	4087	C	MET	534	72.102	10.908	22.785	1.00 31.10	
MOTA	4088	0	MET	534	72.258	10.224	23.791	1.00 32.80	
ATOM	4089	N	MET	535	72.194	10.394	21.563	1.00 30.50	
MOTA	4091	CA	MET	535	72.399	8.961	21.368	1.00 29.25	
ATOM	4092	CB	MET	535	72.577	8.623	19.884	1.00 28.10	
ATOM	4093	CG	MET	535	71.337	8.876	19.042	1.00 27.48	
ATOM	4094	SD	MET	535	71.377	7.980	17.502	1.00 26.94	
ATOM	4095	CE	MET	<b>5</b> 35	71.346	9.275	16.310	1.00 33.72	



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MOTA	4163	CB	LYS	542	68.680	-5.602	21.915	1.00	34.24
MOTA	4164	C	LYS	542	67.674	-3.646	20.802	1.00	32.40
ATOM	4165	0	LYS	542	67.507	-3.822	19.612	1.00	32.37
ATOM	4166	N	ASN	543	66.785	-3.046	21.580	1.00	32.12
ATOM	4168	CA	ASN	543	65.541	-2.561	21.015	1.00	33.01
ATOM	4169	CB	ASN	543	64.361	-3.081	21.842	1.00	
ATOM	4170	CG	ASN	543	64.365	-4.597	21.979	1.00	
ATOM	4171	OD1	ASN	543	64.633	-5.128	23.050		32.23
ATOM	4172		ASN	543	64.077	-5.292	20.904	1.00	
MOTA	4175	Ċ	ASN	543	65.424	-1.050	20.719	1.00	32.21
ATOM	4176	0	ASN	543	64.326	-0.481	20.765		31.13
ATOM	4177	N	ILE	544	66.556	-0.419	20.397	1.00	30.52
ATOM	4179	CA	ILE	544	66.611	1.002	20.028	1.00	29.01
ATOM	4180	CB	ILE	544	67.040	1.962	21.208	1.00	
ATOM	4181	CG2	ILE	544	66.244	1.682	22.467	1.00	
ATOM	4182	CG1	ILE	544	68.532	1.848	21.522	1.00	
ATOM	4183	CD1	ILE	544	69.008	2.839	22.581	1.00	
ATOM	4184	C	ILE	544	67.617	1.118	18.870	1.00	23.49
ATOM	4185	o	ILE	544	68.410	0.194	18.€33	1.00	27.26
MOTA	4186	N	ILE	545	67.504	2.184	18.078		26.74
ATOM	4188	CA	ILE	545	68.453	2.396	16.992		27.06
ATOM	4189	CB	ILE	545	67.913	3.350	15.921		23.64
ATOM	4190	CG2	ILE	545	69.027	3.727	14.955		23.96
ATOM	4191	CG1		545	66.754	2.692	15.167	1.00	23.13
ATOM	4192		ILE	545	67.152	1.481	14.339		20.61
ATOM	4193	C	ILE	545	69.720	2.968	17.633		26.93
ATOM	4194	Ċ	ILE	545	69.719	4.075	18.160		28.63
ATOM	4195	N	ASN	546	70.800	2.200	17.560		28.53
ATOM	4197	CA	ASN	546	72.075	2.567	18.161		29.39
ATOM	4198	СВ	ASN	546	72.752	1.308	18.718		29.14
ATOM	4199	CG	ASN	546	71.908	0.613	19.772		30.21
ATOM	4200		ASN	546	71.804	1.088	20.899		30.74
ATOM	4201		ASN	546	71.290	-0.505	19.406		30.79
ATOM	4204	С	ASN	546	73.034	3.303	17.238		30.78
ATOM	4205	0	ASN	546	73.011	3.126	16.015		33.04
ATOM	4206	N	LEU	547	73.866	4.151	17.837		31.07
ATOM	4208	CA	LEU	547	74.880	4.904	17.101		31.37
MOTA	4209	CB	LEU	547	75.284	6.165	17.875		27.32
ATOM	4210	CG	LEU .	547	76.413	7.032	17.297		24.17
ATOM	4211	CD1		547	75.953	7.768	16.069		18.06
ATOM	4212	CD2	LEU	547	76.864	8.014	18.348		22.50
ATOM	4213	С	LEU	547	76.107	3.999	16.861		33.38
MOTA	4214	0	LEU	547	76.610	3.343	17.789		33.58
MOTA	4215	N	LEU	548	76.543	3.919	15.607	1.00	
ATOM	4217	CA	LEU	548	77.694	3.104	15.259	1.00	
ATOM	4218	CB	LEU	548	77.388	2.244	14.029	1.00	
ATOM	4219	CG	LEU	548	76.148	1.341	14.158	1.00	
ATOM	4220	CD1		548	76.034	0.513	12.906	1.00	
ATOM	4221	CD2		548	76.196	0.436	15.394	1.00	
ATOM	4222	C	LEU	548	78.941	3.965	15.030		33.69
ATOM	4223	0	LEU	548	80.063	3.488	15.167	1.00	
ATOM	4224	N	GLY	549	78.746	5.229	14.675	1.00	
-						J J	_ 1 . 0 , 5	00	24.10

λ ΤΟν	
ATOM 4226 CA GLY 54	9
4227 C CTV	19.0/1 6.126 -
ATOM 4228 O GTT	79.425 7.429 13 020
ATOM 4229 N N.	78.221 7.686 13.700 31.11
4231 Ch 272	80.388 8 360 1 1.00 30.15
ATOM 4232 CB NT 350	80.074 9.540 13.474 1.00 31.02
ATOM 4233 C 7550	79.537 10.536 1.00 29.00
ATOM 1224 550	81 252 13.899 1.00 27 82
ATOM 4225 12 250	82 422 1.00 27 66
ATOM 4227 N CYS 551	12,4/4 1 00 0-
ATOM 4335 CA CYS 551	00.944 10.810 10.984 1 00 25
ATOM 1238 CB CYS 551	01.924 11.540 10.170 1 00 27.61
4239 SG CYS FF	8.680 1 00 25.02
4240 C CYS 567	9.553 8.187 1 00 22.41
4241 O CYS 551	81.583 13.009 10 447
ATOM 4242 N mm	80.569 13.525 9.55
A10M 4244 CA TUD	82.367 13 257 1.00 23.55
ATOM 4245 CB TWO	82.110 15 046 11.303 1.00 23.22
ATOM 4246 OCI WID	82.138 15 215
ATOM 40.5	83 470 17 13.202 1.00 26 50
ATOM 1245 552	81 252 - 13.664 1.00 26 22
ATOM 4250 THR 552	83 134 75 13.886 1.00 26 64
ATOM 107	82 894 17 - 11.090 1.00 27 92
ATOM ADDA GLN 553	11.005 1 00 00
ATOM TEST CA GLN 553	75.473 10.663 1 00 33
ATOM 4254 CB GIN 553	05.355 16.288 10.153 1 00 55
4255 CG GLN =53	15.768 10.763
AUCON 4236 CD GLN 553	15.65= 12.220
TEST OE1 GLN FF3	86.534 17.007 13.00
4258 NEC 37	87.440 17.821 12 000 26.86
4261 C CT	85.421 17.239 13 (75
A10M 4262 0 CIN	85.475 16.316 9 53.
ATOM 4263 N NC	85.221 15 212 - 0.634 1.00 28.30
ATOM 4265 CA NOT 554	85.860 17 480 7.967 1.90 31.00
ATOM 4266 CP 354	86.070 17 735 8.119 1.00 26.89
ATOM 4267 00 554	87 370 17 00 6.695 1.00 27.85
ATTOM	88 534 12 75 6.257 1.00 33 44
Amore ODI ASP 554	89 030 10 7.060 1.00 37 63
ATOM 4270 554	6.763 1 00
ATOM 4375 ASP 554	18.843 8.000 1 00 35
ATOM 487 554	5.715 1 00 5
ATOM AST N GLY 555	03.193 16.518 4.826 1 00 33
ATOM 42/4 CA GLY 555	03.024 17.981 5.842 1 00 00
4275 C GLV 555	02.720 17.694 4.949 1 00 07
A10M 4276 O GLY 555	01.438 17.567 5 7
4277 N PPO 554	81.423 17.795 6 043
ATOM 4278 CD 336	80.338 17 305 1.00 20.20
ATOM 4279 CA PRO 556	80.280 16 750
ATOM 4280 CP PRO	79.039 17.030 3.679 1.00 22.33
ATOM 4281 CC PRO 556	78.154 16.400 5.733 1.00 23.99
ATOM 4282 C 556	79 144 75 22 4.612 1.00 22 41
ATOM 4383 - PRO 556	79 000 15 3.698 1.00 24 36
ATOM 1224 556	79 954 15
ATOM 1257	79.854 15.111 6.934 1 00 20
4286 CA 1.Fii	76.237 16.325 7.896 7 00 20.37
4287 CB 1.Fit 555	78.168 15.471 9.070 1 00 20
33,	77.550 16 225
SSEDIERA	10.225 10.251 1.00 33.20
SSSD/55145, v01	

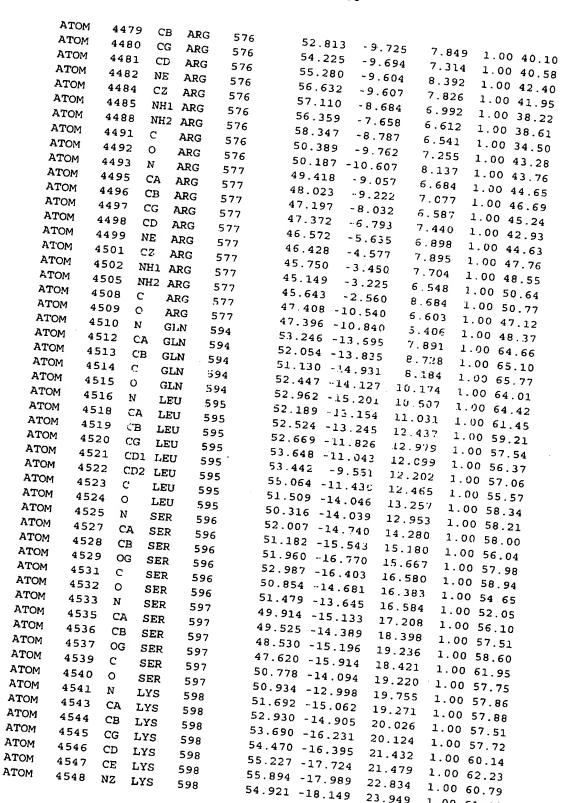
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ATOM	4288	CG	LEU	557	77.109	15.416	11.475	1.00 30.01
MOTA	4289	CD1	LEU	557	78.304	<b>1</b> 4.793	12.174	1.00 29.05
ATOM	4290	CD2	LEU	557	76.365	16.341	12.407	1.00 29.20
ATOM	4291	C	LEU	557	77.324	14.238	8.780	1.00 30.33
ATOM	4292	0	LEU	557	76.175	14.343	8.330	1.00 27.66
MOTA	4293	N	TYR	558	77.913	13.071	9.002	1.00 30.68
ATOM	4295	CA	TYR	558	77.214	11.823	8.812	1.00 29.26
ATOM	4296	CB	TYR	558	77.978	10.933	7.840	1.00 30.99
ATOM	4297	CG	TYR	558	78.066	11.481	6.430	1.00 35.01
ATOM	4298	CD1	TYR	558	79.108	11.109	5.592	1.00 36.17
ATOM	4299	CE1	TYR	558	79.198	11.600	4.296	1.00 41.40
ATOM	4300	CD2	TYR	558	77.109	12.368	5.941	1.00 36.44
ATOM	4301	CE2	TYR	558 .	77.188	12.871	4.648	1.00 40.96
MOTA	4302	CZ	TYR	558	78.237	12.484	3.825	1.00 43.59
ATOM	4303	ОН	TYR	558	78.298	12.965	2.525	1.00 42.91
MOTA	4305	C	TYR	558	77.081	11.125	10.164	1.00 28.18
MOTA	4306	0	TYR	558	78.077	10.855	10.835	1.00 28.06
ATOM	4307	N	VAL	559	75.842	10.879	10.574	1.00 26.72
MOTA	4309	CA	VAL	559	75.548	10.175	11.821	1.00 26.72
MOTA	4310	CB	VAL	559	74.326	10.813	12.552	1.00 28.03
MOTA	4311	CG1	VAL	559	73.915	9.992	13.771	1.00 29.85
ATOM	4312	CG2	VAL	559	74.655	12.236	12.982	1.00 29.37
ATOM	4313	C	VAL	559	75.238	8.723	11.443	1.00 25.58
MOTA	4314	0	VAL	559	74.131	8.402	10.988	1.00 25.73
ATOM	4315	N	ILE	560	76.214	7.851	11.642	1.00 24.35
ATOM	4317	CA	ILE	560	76.061	6.448	11.281	1.00 26.64
ATOM	4318	CB	ILE	560	77.441	5.781	11.002	1.00 26.53
ATOM	4319	CG2	ILE	560	77.252	4.359	10.465	1.00 27.80
MOTA	4320	CG1	ILE	560	78,254	6.620	10.004	1.00 24.69
ATOM	4321	CDI	ILE	560	79.671	6.112	9.763	1.00 17.05
MOTA	4322	C	ILE	560	75.312	5.633	12.339	1.00 27.95
MOTA	4323	0	ILE	560	75.777	5.493	13.479	1.00 25.16
ATOM	4324	N	VAL	561	74.163	5 084	11.951	1.00 27.43
MOTA	4326	CA	VAL	561	73.352	4.265	12.847	1.00 27.69
ATOM	4327	CB	VAL	561	72.048	5.000	13.251	1.00 25.08
MOTA	4328	CG1	VAL	561	72.367	6.302	13.936	1.00 19.97
MOTA	4329		VAL	561	71.186	5.250	12.033	1.00 25.55
ATOM	4330	C	VAL	561	73.031	2.896	12.202	1.00 30.21
MOTA	4331	0	VAL	561	73.404	2.623	11.045	1.00 32.04
ATOM	4332	N	GLU	562	72.306	2.062	12.944	1.00 28.88
MOTA	4334	CA	GLU	562	71.940	0.714	12.509	1.00 27.69
ATOM	4335	CB	GLU	562	71.448	-0.081	13.712	1.00 26.79
ATOM	4336	CG	GLU	562	72.387	0.001	14.873	1.00 28.13
ATOM	4337	CD	GLU	562	72.012	-0.916	16.003	1.00 31.86
ATOM	4338	OE1		562	72.772	-1.876	16.255	1.00 33.17
ATOM	4339		GLU	562	70.974	-0.654	16.639	1.00 35.50
ATOM	4340	C	GLU	562	70.898	0.636	11.405	1.00 27.34
ATOM	4341	0	GLU	562	69.990	1.453	11.358	1.00 29.72
ATOM	4342	N	TYR	563	71.002	-0.392	10.568	1.00 28.07
ATOM	4344	CA	TYR	563	70.080	-0.626	9.455	1.00 32.50
ATOM	4345	CB	TYR	563	70.848	-1.236	8.269	1.00 28.32
ATOM	4346	CG	TYR	563	70.042	-1.427	7.007	1.00 26.56

ATOM 4347 CD1 TYR 56	•
4348 CE1 TYR 56	09.338 -0.378 6 448
ATOM 4349 CD2 TYR 56	68.620 -0.536 5 350 1.00 30.49
ATOM 4350 CE2 TYR 56	70.011 -2.652 6 350
ATOM 4351 CZ TVD 56	69.300 -2.821 5 151 -100 29.07
4352 OH men	68.605 -1.755 4.610
ATOM 4354 C TVD	67.876 -1.919 3 460 33.54
4355 0 mm	68.930 ~1.564 9 977
ATOM 4356 N NT	69.151 -2.569 10.550
ATOM 4358 CD 373	67.711 -1.234 9 454
AIOM 4359 CD 373	66.529 -2.025 9.750
ATOM 4360 C ATA	65.557 -1 207 1.00 38.93
4361 O 313	65.919 -2.360 9 304
4362 N CED -	64.958 -1.736 7 077
ATOM 4364 CA SED SED	66.455 -3.387 7.747 1.00 45.88
ATOM 4365 CB SED 565	66.018 -3.806 6.423
4366 OC CER	66.673 -5.134 = 072
4368 C CED	66.6466.012 7 175
ATOM 4369 0 CER	64.5303.932 6 154
4370 N TYO	64.097 -3.823 5.005
AJOM 4372 CA TVS FEE	63.743 -4.183 7 707
ATOM 4373 CR TVO	62.312 -4.341 = 000 1.00 39.63
ATOM 4374 CC tree	61.807 -5.541 7 703
ATOM 4375 CD 1370	62.468 -6.828 7.300 38.35
A10M 4376 CF TVO	62.161 -8.004 9.300
ATOM 4377 NZ LYS 566	62.734 -9.277 7 603
4381 C LYS 566	62.692 -10.400 8 503
4382 D 1370	61.488 -3.079 7 240
4383 N GLY 567	60.265 -3.132 7 435
4385 CA GTV 55-	62.166 -1.936 7 227
ATOM 4386 C GLY 567	61.497 -0.666 7 422
1387 O GLY 567	51 -0.473 8.761 1 00 31
4388 N ASN 560	50.251 -1.012 9.778 1 00 30 30
TAN SECONO TECONO	59.722 0.294 8.754 1.00 20 25
Amou 4391 CB ASN 568	58.999 0.569 9.974 1.00 31 35
Amore 4392 CG ASN 568	55.414 1.991 9.991 1.00 31.05
ATOM 4393 OD1 ASN 568	55.201 2.157 9.087 1.00 24 15
ATOM 1394 ND2 ASN 568	50.095 1.685 9.385 1.00 27 25
ATOM ASN 568	7.999 1 00 35 15
ATOM ASN 568	100 10.235 1 00 20
ATOM 1150 N LEU 569	57 515 9.324 1.00 31 76
ATOM 1400 569	56 540 11.490 1.00 34 62
ATOM LEU 569	56 454 2.311 11.979 1.00 35 40
7704 4403 CG LEU 569	55 500 13.500 1.00 36 13
7704 CD1 LEU 569	56 010 -2.363 14.210 1.00 34 78
ATOM 1405 CD2 LEU 569	55 435 -3.804 14.034 1.00 35 01
4406 C LEU 560	55 341 -1.971 15.664 1.00 31 13
4407 O LEU 560	54 510 -1.420 11.382 1.00 37 34
ATOM 1408 N ARG 570	54.518 -2.447 11.141 1.00 41 49
ATOM ATOM CA ARG 570	53 200 -0.213 11.162 1.00 37 19
ATOM	52 970 -0.063 10.591 1.00 39 79
ATOM 4412 CG ARG 570	1.403 10.331 1 00 30
	51.558 1.638 9.887 1.00 41.93
SSSD/55145, v01	**.53

MOTA	4413	CD	ARG	570	51.459	2.966	9.182	1.00	49.89
ATOM	4414	NE	ARG	570	52.329	2.991	8.009	1.00	55.25
MOTA	4416	CZ	ARG	570	53.121	4.008	7.693	1.00	57.90
ATOM	4417	NH1	ARG	570	53.145	5.093	8.455	1.00	56.93
ATOM	4420	NH2	ARG	570	53.921	3.920	6.637	1.00	57.58
MOTA	4423	C	ARG	570	53.219	-0.835	9.278	1.00	39.84
MOTA	4424	0	ARG	570	52.309	-1.644	9.060	1.00	42.48
ATOM	4425	N	GLU	571	54.208	-0.597	8.425	1.00	38.22
ATOM	4427	CA	GLU	571	54.292	-1.251	7.135	1.00	38.84
MOTA	4428	CB	GLU	571	55.284	-0.492	6.266	1.00	40.72
MOTA	4429	CG	GLU	571	54.818	0.941	5.999	1.00	49.17
ATOM	4430	CD	GLU	571	55.845	1.798	5.284	1.00	58.95
MOTA	4431	OE1	GLU	571	57.047	1.434	5.278	1.00	67.07
MOTA	4432	OE2	GLU	571	55.455	2.854	4.736	1.00	61.02
MOTA	4433	C	GLU	571	54.617	-2.744	7.240	1.00	37.79
ATOM	4434	C	GLU	571	54.075	-3.558	6.488	1.00	37.63
ATOM	4435	N	TYR	572	55.462	-3.104	8.204	1.00	36.89
MOTA	4437	CA	TYR	572	55.841	-4.498	8.437	1.00	36.81
MOTA	4438	CB	TYR	572	56.822	-4.584	9.612	1.00	33.24
MOTA	4439	CG	TYR	572	57.191	-5.987	10.080	1.00	33.42
MOTA	4440	CD1	TYR	572	58.209	-6.714	9.450	1.00	31.93
· ATOM	4441	CE1	TYR	572	58.623	-7.960	9.936	1.00	30.14
ATOM	4442	CD2		572	56586	-6.552	11.208	1.00	34.42
ATOM	4443	CE2	TYR	572	56.991	-7.799	11.704	1.00	32.29
MOTA	4444	CZ	TYR	572	58.012	-8.495	11.065	1.00	32.52
MOTA	4445	ОН	TYR	572	58.427	-9717	11.571	1.00	31.70
MOTA	4447	C	TYR	572	54.588	-5.310	8.754	1.00	37.64
ATOM	4448	0	TYR	572	54.387	-6.410	8.226	1.00	35.70
ATOM	4449	N	LEU	573	53.742	-4.740	9.608		38.63
MOTA	4451	CA	LEU	573	52.498	-5.376	10.011	1.00	38.21
ATOM	4452	CB	LEU	573	51.802	-4.532	11.067		35.40
ATOM	4453	CG	LEU	573	52.494	-4.421	12.419		34.55
ATOM	4454		LEU	573	51.755	-3.402	13.258		32.02
ATOM	4455			573	52.537	-5.788	13.108		34.58
ATOM	4456	C	LEU	573	51.570	-5.549	8.818		38.11
ATOM	4457	0	LEU	573	51.144	-6.656	8.507		37.68
MOTA	4458	N	GLN	574	51.286	-4.448	8.138		40.92
MOTA MOTA	4460	CA	GLN	574	50.402	-4.476	6.982		45.16
	4461	CB	GLN	574 574	50.213	-3.071	6.447		44.16
ATOM ATOM	4462	CG	GLN	574	49.380	-2.239	7.369		45.26
ATOM	4463	CD OE1	GLN	574	49.222	-0.849	6.863	1.00	
ATOM	4464		GLN GLN	574	49.789	-0.483	5.838	1.00	
ATOM	4465 4468	C		574 574	48.450	-0.051	7.573	1.00	
MOTA	4469		GLN	574 574	50.807	-5.419	5.861	1.00	
ATOM	4470	O N	GLN	574 575	49.951	-6.031	5.215	1.00	
MOTA			ALA	575	52.105	-5.562	5.646	1.00	
ATOM	4472 4473	CA CB	ALA	575 575	52.579	-6.446	4.604	1.00	
ATOM	4474	CB	ALA	575 576	54.023	-6.130	4.284	1.00	
ATOM		. 0	ALA	575 575	52.439	-7.906	5.022	1.00	
ATOM	4476		ALA	575 576	52.771	-8.804	4.254	1.00	
ATOM	4478	N CA	ARG ARG	576	51.937	-8.142	6.229	1.00	
-11 OF	77 / O	CM	MRG	576	51.787	-9.494	6.747	1.00	41.58



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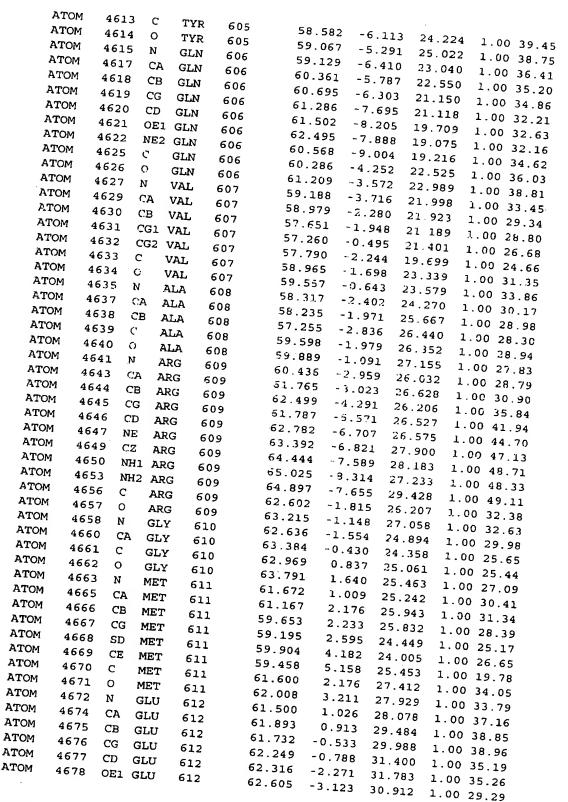
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					12 829 19.389 1.00 55.94
				598	53.809 -13.827 1 00 55 84
MOTA		_	LYS	598	54.322 -12.955 20.089 1.00 53 32
MOTA	4553	0	LYS	599	53.935 -13.866 18.061 1.00 50.30
MOTA	4554	N	ASP	599	54.737 -12.882 17.334 1.00 49 72
MOTA	4556	ÇA	ASP	599	54.688 -13.119 15.823 1.00 53 97
MOTA	4557	CB	ASP	599	55.426 -14.383 15.394 1.00 58 12
MOTA	4558	CG	ASP	599 5 <b>9</b> 9	56.176 -14 948 16.214 1.00 55 58
MOTA	4559		ASP	599	55.261 -14.822 14.233 1.00 33.00
MOTA	4560		ASP	599	54.247 -11.474 17.636 1.00 13.16
ATOM	4561	С	ASP	599	55.054 -10.589 17.911 1.00 32-50
MOTA	4562	0	ASP	600	52.930 -11.281 17.634 1.00 15.41
MOTA	4563	N	LEU	600	52.354 -9.972 17.909 1.00 43.77
MOTA	4565	CA	LEU	600	50.850 -9.948 17.627 1.00 12
MOTA	4566	CB	LEU	600	50.429 -10.121 16.165 1.00 41 04
MOTA	4567	CG	LEU	600	48.941 -9 904 16.048 1.00 29 59
MOTA	4568	CD:	LEU	600	51.160 -9 140 15.294 1.00 25
MOTA	4569		2 LEU	600	52.638 -9.485 19.318 1.00 48 74
MOTA	4570	C	LEU	600	52.964 -8.308 19.497 1.00
MOTA	4571	0	LEU	601	52.524 -10.372 20 314 1.00 47 38
MOTA	4572		VAL	601	52.804 -10.002 21.716 1.00 1.58
MOTA	4574			601	52.321 -11.070 22.756 1.00 45 07
MOTA	4575			601	52.081 -10.403 24.114 1.00 48 86
MOTA	4576		1 VAL	601	51.058 -11.759 22.306 1.00 46 04
MOTA			2 VAL	601	54.321 -9.511 22-1 20.46 13
MOTA		_	JAV		54.793 -8.935 22.622 1.00 44 23
MOTA					55.090 -10.624 21.183 1.00 278
MOTA					56.534 -10.540 22 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
MOTA					57.119 -11.594 40.51 00 51 02
ATOM		_			58.52311.613 20.012 1 00 41.74
MOTA					56.954 -9.133 20.524 1 00 44.09
ATOM		_			57.709 28.407 22 605 1 00 39.57
ATON				·	56.425 -8.507 -2 177 1 00 36.11
OTA		•	A CY		56.699 -7.317 27.024 1 00 34.72
IOTA		_	B CY		55.852 -7.038 17.323 0 50 29.10 PRT1
ATO		-	SG CY		55.760 -5.364 27.00 34.50
OTA			C CY		56.378 -6.272 20.506 1.00 33.61
ATO			O CY		57.174 -5.371 20.913 1.00 34.64
OTA			N AL		55.236 -6.425 - 01.064 1.00 37.18
ATC			CA AI		54.811 -5.300 22 414 1 00 38.20
OTA			CB AI		53.386 -5.830 22 260 1 00 38.91
ATO		99		A 604	55.786 -5.310 -5.700 3.00 38.29
ATO		00	•	A 604	56.026 -4.401 1 00 39.54
TA		01	-	YR 605	56.323 -6.695 24.565 1.00 39.29
ATO	···	503		YR 605	57.283 -6.834 24 701 1 00 40.07
TA		504		YR 605	57.573 -8.532 25.807 1.00 39.09
	-	605		YR 605	58.663 -8.022 23.137 1.00 38.50
		606	CD1 T		58.525 -8.230 274 1.00 40.76
		607		YR 605	59.526 -8.503 25.435 1.00 39.73
		608		YR 605	59.831 -9.263 25.361 1.00 37.45
		609		YR 605	60.834 29.335 27.677 1.00 40.34
	- ·	610		TYR 605	60.678 -3.166 29 601 1.00 43.16
		611		ryr 605	
A	TOM 4				

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ATOM	4679	OE2	GLU	612	62.102	-2.588	32.982	1.00 37.85
MOTA	4680	С	GLU	612	63.353	1.364	29.628	1.00 40.01
ATOM	4681	0	GLU	612	63.720	2.060	30.584	1.00 38.27
ATOM	4682	N	TYR	613	64.176	0.972	28.662	1.00 40.33
ATOM	4684	CA	TYR	613	65.575	1.362	28.664	1.00 39.71
ATOM	4685	CB	TYR	613	66.333	0.722	27.494	1.00 39.03
ATOM	4686	CG	TYR	613	67.800	1.100	27.467	1.00 41.41
ATOM	4687	CD1	TYR	613	68.702	0.527	28.364	1.00 42.79
ATOM	4688	CE1	TYR	613	70.048	0.905	28.386	1.00 40.21
ATOM	4689	CD2	TYR	613	68.283	2.068	26.581	1.00.39.75
MOTA	4690	CE2	TYR	613	69.621	2.454	26.596	1.00 39.01
ATOM	4691	CZ	TYR	613	70.499	1.868	27.503	1.00 39.56
ATOM	4692	ОН	TYR	613	71.823	2.249	27.538	1.00 35.63
ATOM	4694	C	TYR	613	65.642	2.881	28.562	1.00 38.71
ATOM	4695	0	TYR	613	66.106	3.541	29.486	1.00 38.52
ATOM	4696	N	LEU	614	65.126	3.423	27.460	1.00 37.22
ATOM	4698	CA	LEU	614	65.128	4.864	27.212	1.00 35.66
ATOM	4699	CB	LEU	614	64.223	5.202	26.025	1.00 35.27
MOTA	4700	CG	LEU	614	64.687	4.699	24.659	1.00 33.09
ATOM	4701		LEU	614	63.718	·5188	23.612	1.00 33.31
ATOM	4702	CD2	LEU	614	66.099	5.184	24.363	1.00 31.20
ATOM	4703	C	LEU	614	64.672	5.653	28.430	1.00 35.64
ATOM	4704	0	LEU	614	65.298	6.639	28.816	1.00 34.54
ATOM	4705	N	ALA	615.	63.577	5.203	29.032	1.00 36.61
ATOM	4707	CA	ALA	615	63.028	5.835	30.222	1.00 37.74
ATOM	4708	CB	ALA	615	61.682	.5.187	30.60Ŗ	1.00 37.74
ATOM	4709	С	ALA	615	64.021	5.776	31.389	1.00 37.30
ATOM	4710	0	ALA	615	64.111	6.731	32.175	1.00 37.29
ATOM	4711	N	SER	616	64.752	4.665	31.511	1.00 37.18
ATOM	4713	CA	SER	616	65.741	4.534	32.577	1.00 36.92
ATOM	4714	CB	SER	616	66.274	3.091	32.702	1.00 34.82
ATOM	4715	OG	SER	616	67.106	2.680	31.628	1.00 28.79
ATOM	4717	C	SER	616	66.870	5.516	32.287	1.00 38.57
ATOM	4718	0	SER	616	67.633	5.902	33.179	1.00 38.30
ATOM	4719	N	LYS	617	66.958	5.925	31.024	1.00 37.62
ATOM	4721	CA	LYS	617	67.965	6.876	30.606	1.00 36.13
ATOM ATOM	4722	CB	LYS	617	68.511	6.494	29.238	1.00 35.90
	4723	CG	LYS	617	69.274	5.206	29.236	1.00 34.58
ATOM	4724	CD	LYS	617	70.502	5.348	30.077	1.00 35.44
ATOM	4725	CE	LYS	617	71.201	4.022	30.232	1.00 38.54
ATOM	4726	NZ	LYS	617	72.566	4.211	30.790	1.00 41.54
ATOM	4730	С	LYS	617	67.378	8.275	30.564	1.00 36.55
ATOM	4731	0	LYS	617	67.943	9.155	29.934	1.00 40.26
ATOM	4732	N	LYS	618	66.221	8.468	31.187	1.00 36.42
ATOM	4734	CA	LYS	618	65.570	9.779	31.231	1.00 36.06
ATOM	4735	CB	LYS	618	66.543	10.833	31.746	1.00 42.22
ATOM	4736		LYS	618	67.234	10.499	33.062	1.00 52.36
ATOM	4737	CD	LYS	618	66.301	10.668	34.236	1.00 61.51
ATOM	4738		LYS	618	66.933	10.121	35.495	1.00 67.28
ATOM	4739	NZ	LYS	618	65.965	10.161	36.618	1.00 73.99
ATOM	4743		LYS	618	65.026	10.261	29.887	1.00 34.94
ATOM	4744	0	LYS	618	64.562	11.393	29.781	1.00 34.69

ATOM 4745 N CYS 619 65.051 9.407 28.872 1.00 34.46 ATOM 4740 CR CYS 619 64.588 9.793 27.543 1.00 33.12 ATOM 4740 7479 SG CYS 619 64.920 9.397 24.778 1.00 34.33 ATOM 4750 C CYS 619 64.920 9.397 24.778 1.00 34.33 ATOM 4751 O CYS 619 64.920 9.397 24.778 1.00 32.13 ATOM 4751 O CYS 619 62.465 8.645 27.584 1.00 32.13 ATOM 4751 O CYS 619 62.465 8.645 27.584 1.00 32.13 ATOM 4752 N ILE 620 62.477 10.818 26.966 1.00 32.70 ATOM 4755 CR ILE 620 62.477 10.818 26.966 1.00 32.75 ATOM 4755 CR ILE 620 60.440 12.129 27.421 1.00 33.55 ATOM 4757 CGI ILE 620 60.440 12.129 27.421 1.00 33.53 ATOM 4757 CGI ILE 620 60.446 11.913 28.983 1.00 30.71 ATOM 4758 CDI ILE 620 60.486 11.913 28.983 1.00 30.71 ATOM 4758 CDI ILE 620 60.486 11.913 28.983 1.00 30.71 ATOM 4758 CDI ILE 620 60.486 11.913 28.993 1.00 30.71 ATOM 4763 O ILE 620 60.969 11.006 22.700 1.00 33.35 ATOM 4763 CR ILE 620 60.486 11.913 28.993 1.00 30.71 ATOM 4763 CR ILE 620 60.496 12.009 22.008 1.00 33.35 ATOM 4763 CR ILE 620 60.496 12.009 23.087 1.00 33.36 ATOM 4764 CR HIS 621 60.250 10.009 23.087 1.00 33.36 ATOM 4764 CR HIS 621 60.250 10.009 23.087 1.00 32.75 ATOM 4766 CD HIS 621 59.866 8.668 22.642 1.00 29.55 ATOM 4766 CD HIS 621 59.866 8.668 22.642 1.00 29.55 ATOM 4767 NDI HIS 621 59.866 8.668 22.642 1.00 29.55 ATOM 4769 CR HIS 621 59.464 11.00 33.31 1.00 32.70 ATOM 4769 CR HIS 621 59.464 11.00 32.495 11.00 32.70 ATOM 4769 CR HIS 621 59.464 11.00 32.495 11.00 32.30 ATOM 4779 CR ARG 622 58.137 11.02 32.495 11.00 32.495 11.00 32.665 ATOM 4779 CR ARG 622 57.594 11.103 32.495 11.00 32.495 11.00 32.665 ATOM 4779 CR ARG 622 58.138 11.363 31.79 1.00 32.665 ATOM 4779 CR ARG 622 58.138 11.363 31.79 1.00 32.65 ATOM 4789 CR ARG 622 58.618 11.363 31.79 1.00 32.66 ATOM 4789 CR ARG 622 58.618 11.363 11.00 32.495 1.00 33.79 ATOM 4790 CR ARG 622 58.618 11.363 11.00 32.495 1.00 32.62 ATOM 4790 CR ARG 622 58.618 11.363 11.00 32.495 1.00 32.62 ATOM 4790 CR ARG 622 55.597 11.00 22.135 1.00 32.70 ATOM 4790 CR ARG 622 55.597 11.00 22.135 1.00 32.70 ATOM 4790 CR ARG 622 55.597 11.00 22.135 1.00 32.7	) many	
ATOM 4749 CB CYS 619 ATOM 4749 SG CYS 619 ATOM 4749 SG CYS 619 ATOM 4750 C CYS 619 ATOM 4751 O CYS 619 ATOM 4751 O CYS 619 ATOM 4752 N ILE 620 ATOM 4755 CB ILE 620 ATOM 4755 CC ILE 620 ATOM 4756 CCI ILE 620 ATOM 4756 CCI ILE 620 ATOM 4758 CDI ILE 620 ATOM 4758 CDI ILE 620 ATOM 4760 O ILE 620 ATOM 4761 N HIS 621 ATOM 4761 CB HIS 621 ATOM 4765 CB HIS 621 ATOM 4766 CD HIS 621 ATOM 4767 NDI HIS 621 ATOM 4767 NDI HIS 621 ATOM 4767 NDI HIS 621 ATOM 4768 CB HIS 621 ATOM 4768 CB HIS 621 ATOM 4769 CB HIS 621 ATOM 4760 NDI HIS 621 ATOM 4766 CD HIS 621 ATOM 4767 NDI HIS 621 ATOM 4767 NDI HIS 621 ATOM 4768 CB HIS 621 ATOM 4768 CB HIS 621 ATOM 4769 NDI HIS 621 ATOM 4769 CB HIS 621 ATOM 4769 NDI HIS 621 ATOM 4769 CB HIS 621 ATOM 4769 CB HIS 621 ATOM 4769 NDI HIS 621 ATOM 4769 CB HIS 621 ATOM 4769 CB HIS 621 ATOM 4769 NDI HIS 621 ATOM 4769 CB HIS 621 ATOM 4769 CB HIS 621 ATOM 4769 NDI HIS 621 ATOM 4760 NDI HIS 621 ATOM		9
ATOM 4748 CB CKS 619 65.311 8.966 26.475 1.00 33.12 ATOM 4750 C CYS 619 64.920 9.397 24.778 1.00 35.64 ATOM 4751 C CYS 619 66.920 9.397 24.778 1.00 35.64 ATOM 4752 N ILE 620 62.465 8.645 27.554 1.00 32.75 ATOM 4754 CA ILE 620 62.465 8.645 27.554 1.00 32.75 ATOM 4755 CG ILE 620 61.046 10.909 26.708 1.00 32.75 ATOM 4756 CG2 ILE 620 60.440 12.129 27.421 1.00 33.55 ATOM 4758 CD1 ILE 620 60.440 12.129 27.421 1.00 33.55 ATOM 4758 CD1 ILE 620 60.440 12.129 27.421 1.00 33.55 ATOM 4758 CD1 ILE 620 60.466 11.913 28.993 1.00 30.71 ATOM 4760 0 ILE 620 60.969 11.086 25.206 1.00 30.71 ATOM 4761 N HIS 621 60.356 10.114 24.533 1.00 33.56 ATOM 4762 CB HIS 621 60.236 10.142 24.533 1.00 33.56 ATOM 4764 CB HIS 621 60.236 10.142 24.533 1.00 33.56 ATOM 4765 CD2 HIS 621 60.049 8.402 21.733 1.00 33.56 ATOM 4766 ND1 HIS 621 60.049 8.402 21.73 1.00 23.30 ATOM 4767 ND1 HIS 621 60.049 8.402 21.73 1.00 23.30 ATOM 4767 ND1 HIS 621 60.049 8.402 21.73 1.00 25.20 ATOM 4769 CEH HIS 621 60.049 8.402 21.73 1.00 25.20 ATOM 4769 CEH HIS 621 60.049 8.402 21.73 1.00 25.20 ATOM 4769 CEH HIS 621 60.049 8.402 21.73 1.00 25.20 ATOM 4769 ND1 HIS 621 60.049 8.402 21.73 1.00 25.20 ATOM 4769 ND1 HIS 621 60.049 8.402 21.73 1.00 25.20 ATOM 4779 NSE HIS 621 60.049 8.402 21.73 1.00 25.20 ATOM 4779 C HIS 621 59.734 8.652 19.006 1.00 25.20 ATOM 4779 C HIS 621 59.462 9.173 20.187 1.00 26.65 ATOM 4779 C HIS 622 58.171 14.253 23.937 1.00 33.79 ATOM 4779 C ARG 622 58.171 14.253 23.937 1.00 36.40 ATOM 4780 NE ARG 622 58.171 14.253 23.937 1.00 35.62 ATOM 4799 C ARG 622 55.575 1.59 1.50 36.40 ATOM 4799 C ARG 622 55.577 1.10 1.02 2.668 1.00 36.40 ATOM 4799 C ARG 622 55.577 1.10 1.02 2.581 1.00 25.20 ATOM 4790 NE ARG 622 55.577 1.10 1.02 2.581 1.00 36.23 ATOM 4790 C ARG 622 55.577 1.10 1.02 2.581 1.00 35.64 ATOM 4790 C ARG 622 56.664 1.00 38 1.00 35.64 ATOM 4790 C ARG 622 56.664 1.00 38 1.00 35.64 ATOM 4790 C ARG 622 56.664 1.00 38 1.00 35.64 ATOM 4790 C ARG 623 56.679 1.00 32.79 1.00 31.71 ATOM 4796 DIASP AG 624 56.079 1.00 32.79 1.00 31.71 ATOM 4796 DIASP AG 624 56.079 1	ATOM 4747 CA CYS 61	9.407 29 873
ATOM 4749 SG CVS 619 64.920 9.397 24.778 1.00 34.33 ATOM 4751 O CVS 619 63.075 9.699 27.355 1.00 35.64 ATOM 4752 N ILE 620 62.465 8.645 27.584 1.00 30.72 ATOM 4755 CB ILE 620 61.046 10.999 26.708 1.00 32.75 ATOM 4755 CB ILE 620 60.440 12.129 27.421 1.00 33.55 ATOM 4757 CG1 ILE 620 60.440 12.129 27.421 1.00 33.55 ATOM 4758 CD1 ILE 620 60.486 11.913 28.933 1.00 30.71 ATOM 4758 CD1 ILE 620 60.486 11.913 28.933 1.00 30.71 ATOM 4760 N ILE 620 60.969 11.086 25.206 1.00 30.71 ATOM 4761 N HIS 621 60.356 10.114 24.553 1.00 30.71 ATOM 4763 CA HIS 621 60.356 10.114 24.553 1.00 33.55 ATOM 4766 CD2 HIS 621 60.049 8.402 21.173 1.00 22.35 ATOM 4766 CD2 HIS 621 60.049 8.402 21.173 1.00 27.32 ATOM 4767 ND1 HIS 621 60.069 8.402 21.173 1.00 27.32 ATOM 4767 ND1 HIS 621 60.069 8.402 21.173 1.00 27.32 ATOM 4767 CR HS 621 60.491 8.602 9.703 1.00 32.30 ATOM 4769 CE1 HIS 621 60.049 8.402 21.173 1.00 27.32 ATOM 4767 ND1 HIS 621 60.049 8.402 21.173 1.00 27.32 ATOM 4767 ND1 HIS 621 60.049 8.402 21.173 1.00 27.32 ATOM 4767 CR ARG 622 59.734 8.652 9.006 1.00 36.39 ATOM 4770 CR HS 621 621 622 60.481 7.579 19.184 1.00 36.39 ATOM 4770 CR ARG 622 59.459 11.574 21.388 1.00 36.39 ATOM 4777 CR ARG 622 59.459 11.574 21.388 1.00 36.39 ATOM 4778 CR ARG 622 57.694 13.732 22.686 1.00 36.39 ATOM 4779 CR ARG 622 57.694 13.732 22.687 1.00 33.79 ATOM 4780 NR ARG 622 58.171 14.253 3.337 1.00 33.79 ATOM 4798 CR ARG 622 57.694 13.732 22.687 1.00 35.64 ATOM 4799 CR ARG 622 58.171 14.253 3.337 1.00 33.79 ATOM 4799 CR ARG 622 57.694 13.732 22.687 1.00 35.64 ATOM 4799 CR ARG 622 57.694 13.732 22.687 1.00 35.64 ATOM 4799 CR ARG 622 57.694 13.732 22.687 1.00 35.62 ATOM 4799 CR ARG 622 58.171 14.253 3.3377 1.00 33.79 ATOM 4799 CR ARG 622 58.171 14.253 3.3377 1.00 33.79 ATOM 4799 CR ARG 622 58.171 14.253 3.3377 1.00 33.79 ATOM 4799 CR ARG 622 58.171 14.253 3.3377 1.00 33.79 ATOM 4799 CR ARG 622 58.171 14.253 3.3377 1.00 33.79 ATOM 4799 CR ARG 622 58.171 14.253 3.3377 1.00 33.79 ATOM 4799 CR ARG 622 58.6405 12.008 21.355 1.00 36.29 ATOM 4799 CR ARG 623 56.640 10.093 2	ATUM 4748 CB CVC	9.793 27 543
ATOM 4750 C CYS 619 63.075 9.699 27.355 1.00 35.64 ATOM 4751 N ILE 620 62.465 8.645 27.584 1.00 32.13 ATOM 4754 CA ILE 620 62.477 10.818 26.960 1.00 32.75 ATOM 4755 CG ILE 620 60.440 12.129 27.421 1.00 33.55 ATOM 4756 CG2 ILE 620 60.440 12.129 26.708 1.00 32.75 ATOM 4757 CG1 ILE 620 60.440 12.129 26.986 1.00 32.75 ATOM 4758 CG2 ILE 620 60.440 12.129 26.986 1.00 32.75 ATOM 4759 C ILE 620 60.486 11.913 28.993 1.00 30.71 ATOM 4759 C ILE 620 60.486 11.913 28.993 1.00 30.71 ATOM 4761 N HIS 621 60.969 11.086 25.206 1.00 33.31 ATOM 4762 CB HIS 621 60.356 10.114 42.533 1.00 33.55 ATOM 4765 CG HIS 621 60.356 10.114 42.533 1.00 33.56 ATOM 4765 CG HIS 621 60.230 10.092 23.087 1.00 32.75 ATOM 4766 CD HIS 621 60.694 7.404 26.533 1.00 25.55 ATOM 4767 ND1 HIS 621 60.694 7.404 26.533 1.00 25.20 ATOM 4769 CD HIS 621 60.694 7.404 26.533 1.00 25.20 ATOM 4760 CD HIS 621 60.694 7.404 26.533 1.00 25.20 ATOM 4760 CD HIS 621 60.694 7.404 26.533 1.00 25.20 ATOM 4760 CD HIS 621 60.694 7.404 26.533 1.00 25.20 ATOM 4760 CD HIS 621 60.694 7.404 26.533 1.00 25.20 ATOM 4770 NEZ HIS 621 60.694 7.404 26.533 1.00 25.20 ATOM 4770 NEZ HIS 621 60.481 7.579 19.184 1.00 25.80 ATOM 4770 CB HIS 621 59.734 8.652 19.006 1.00 25.20 ATOM 4770 NEZ HIS 621 59.748 8.652 19.006 1.00 25.20 ATOM 4770 C HIS 621 59.749 11.362 21.379 1.00 35.40 ATOM 4777 C A ARG 622 57.117 12.323 22.686 1.00 36.39 ATOM 4778 C A ARG 622 57.117 12.323 22.686 1.00 36.39 ATOM 4790 C ARG 622 57.117 12.323 22.686 1.00 35.40 ATOM 4791 N ASP 623 56.605 12.008 21.355 1.00 36.79 ATOM 4792 C ARG 622 57.117 12.323 22.686 1.00 35.81 ATOM 4793 C ARG 622 57.117 12.323 22.686 1.00 35.81 ATOM 4794 C B ASP 623 56.605 12.008 21.355 1.00 35.68 ATOM 4799 C ARG 622 57.117 12.323 22.617 1.00 35.62 ATOM 4799 C ARG 622 57.117 12.323 22.617 1.00 35.62 ATOM 4799 C ARG 622 57.117 12.323 22.617 1.00 35.62 ATOM 4799 C ARG 622 57.117 12.323 22.617 1.00 35.62 ATOM 4799 C ARG 622 57.117 12.323 22.617 1.00 35.62 ATOM 4799 C ARG 622 57.117 12.323 22.617 1.00 35.64 ATOM 4799 C ARG 622 57.117 12.323 22.617 1.00 35.62	ATOM 4749 SG (740	65.311 8.966 26 475
ATOM 4751 0 CS 619 63.075 9.699 27.355 1.00 35.64 ATOM 4752 N ILE 620 62.467 10.818 27.584 1.00 32.13 ATOM 4755 CB ILE 620 62.477 10.818 26.960 1.00 32.75 ATOM 4755 CB ILE 620 60.440 10.909 26.708 1.00 32.75 ATOM 4757 CGI ILE 620 60.440 12.129 27.11 1.00 33.56 ATOM 4758 CDI ILE 620 60.460 11.913 28.933 1.00 38.39 ATOM 4758 CDI ILE 620 60.460 11.913 28.933 1.00 30.71 ATOM 4760 O ILE 620 60.969 11.086 25.206 1.00 33.31 ATOM 4761 N HIS 621 60.366 10.919 23.087 1.00 33.36 ATOM 4763 CA HIS 621 60.356 10.114 24.533 1.00 33.56 ATOM 4765 CD HIS 621 60.366 8.668 22.642 1.00 33.36 ATOM 4766 CD2 HIS 621 60.366 8.668 22.642 1.00 29.55 ATOM 4766 CD2 HIS 621 60.694 7.404 20.573 1.00 27.32 ATOM 4767 CG HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4769 CEI HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4770 NP2 HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4770 NP2 HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4776 CA ARG 622 58.818 11.63 21.393 7.00 25.20 ATOM 4776 CA ARG 622 57.694 13.03 22.499 1.00 36.39 ATOM 4776 CA ARG 622 58.818 11.63 23.378 1.00 36.39 ATOM 4776 CA ARG 622 57.694 13.732 22.686 1.00 36.40 ATOM 4779 CB ARG 622 57.694 13.732 22.677 1.00 33.31 ATOM 4776 CA ARG 622 58.818 11.363 23.378 1.00 35.40 ATOM 4779 CB ARG 622 57.694 13.732 22.677 1.00 33.37 ATOM 4779 CD ARG 622 57.694 13.732 22.677 1.00 33.37 ATOM 4779 CD ARG 622 58.817 14.253 23.937 1.00 35.40 ATOM 4780 NE ARG 622 58.817 14.253 23.937 1.00 35.62 ATOM 4780 NE ARG 622 58.817 14.253 23.937 1.00 35.04 ATOM 4780 NE ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4799 O ARG 623 56.606 12.008 10.00 25.81 ATOM 4799 O ARG 623 56.607 12.008 21.355 1.00 35.64 ATOM 4799 O ARG 623 56.607 12.008 21.35 1.00 35.64 ATOM 4798 C ARG 623 56.77 12.763 20.991 1.00 35.04 ATOM 4800 N LEU 624 56.009 6.801 12.009 1.00 31.71 ATOM 4800 C LEU 624 56.009 6.801 12.009 1.00 31.71 ATOM 4800 C LEU 624 56.009 6.801 12.009 1.00 31.71 ATOM 4800 C DLEU 624 56.009 6.801 12.009 1.00 31.71 ATOM 4800 C DLEU 624 56.009 6.801 12.009 1.00 31.71	ATOM 4750 C CVC	64.920 9.397 24 770
ATOM 4752 N ILE 620 62.477 10.818 26.960 1.00 30.72  ATOM 4755 CB ILE 620 61.046 10.909 26.708 1.00 32.70  ATOM 4756 CG2 ILE 620 60.440 12.129 27.421 1.00 33.55  ATOM 4758 CD1 ILE 620 60.440 12.129 27.421 1.00 33.55  ATOM 4759 C ILE 620 60.440 12.129 27.421 1.00 33.55  ATOM 4759 C ILE 620 60.446 11.913 28.931 1.00 30.71  ATOM 4760 O ILE 620 60.969 11.086 25.206 1.00 30.11  ATOM 4761 N HIS 621 60.356 10.114 24.533 1.00 30.11  ATOM 4762 CB HIS 621 59.866 8.668 22.642 1.00 33.36  ATOM 4765 CC HIS 621 59.866 8.668 22.642 1.00 29.55  ATOM 4766 CD2 HIS 621 60.049 8.402 21.173 1.00 22.52  ATOM 4767 ND1 HIS 621 60.694 7.404 20.533 1.00 24.26  ATOM 4770 NE2 HIS 621 60.481 7.579 19.184 1.00 25.20  ATOM 4771 N NE2 HIS 621 60.481 7.579 19.184 1.00 26.65  ATOM 4772 C HIS 621 60.481 7.579 19.184 1.00 26.65  ATOM 4773 U HIS 621 62.463 22.499 1.00 35.40  ATOM 4773 C R R R G 622 57.694 13.732 22.617 1.00 33.40  ATOM 4773 C R R R G 622 57.117 12.323 22.686 1.00 39.18  ATOM 4778 C R R R G 622 57.117 12.323 22.686 1.00 39.18  ATOM 4779 C R R R G 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.62  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.79  ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17  ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17  ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 35.64  ATOM 4780 C ARG 622 56.405 12.008 21.355 1.00 35.64  ATOM 4780 NE ARG 622 60.487 15.786 25.759 0.50 33.44  ATOM 4780 NE ARG 622 60.487 15.786 25.759 0.50 33.44  ATOM 4780 NE ARG 622 60.487 15.786 25.759 0.50 33.74  ATOM 4780 C ARG 622 56.405 12.008 21.355 1.00 35.6	ATOM 4751 0	63.075
ATOM 4754 CA ILE 620 62.477 10.818 26.960 1.00 32.70 ATOM 4755 CB ILE 620 61.046 10.909 26.708 1.00 32.75 ATOM 4755 CG2 ILE 620 60.440 12.129 27.421 1.00 32.75 ATOM 4757 CG1 ILE 620 59.002 12.139 26.986 1.00 38.39 ATOM 4758 CD1 ILE 620 59.994 13.084 29.710 1.00 38.39 ATOM 4760 O ILE 620 60.468 11.913 28.933 1.00 30.71 ATOM 4761 N HIS 621 60.566 10.114 24.674 1.00 33.31 ATOM 4763 CA HIS 621 60.356 10.114 24.533 1.00 33.31 ATOM 4764 CB HIS 621 60.356 10.114 24.533 1.00 33.30 ATOM 4766 CD2 HIS 621 60.694 7.404 27.533 1.00 32.30 ATOM 4766 CD2 HIS 621 60.694 7.404 20.533 1.00 27.32 ATOM 4767 ND1 HIS 621 60.694 7.404 20.533 1.00 27.32 ATOM 4769 CE1 HIS 621 60.694 7.404 20.533 1.00 27.32 ATOM 4770 NEZ HIS 621 59.866 8.688 22.662 1.00 27.32 ATOM 4770 NEZ HIS 621 59.462 9.173 20.187 1.00 27.32 ATOM 4770 NEZ HIS 621 59.462 9.173 20.187 1.00 26.65 ATOM 4771 N ARG 622 58.128 11.103 22.499 1.00 35.40 ATOM 4777 CB ARG 622 58.128 11.103 22.499 1.00 36.39 ATOM 4776 CA ARG 622 58.128 11.103 22.499 1.00 36.40 ATOM 4779 CD ARG 622 58.128 11.103 22.499 1.00 36.40 ATOM 4779 CD ARG 622 58.128 11.103 22.499 1.00 36.40 ATOM 4780 C ARG 622 58.128 11.103 22.499 1.00 36.40 ATOM 4780 C ARG 622 58.121 1.223 22.617 1.00 33.79 ATOM 4780 C ARG 622 58.121 1.103 22.499 1.00 36.40 ATOM 4780 C ARG 622 58.121 1.103 22.499 1.00 36.40 ATOM 4780 C ARG 622 58.128 11.103 22.499 1.00 36.40 ATOM 4780 C ARG 622 58.121 1.103 22.500 0.50 32.17 ATOM 4780 C ARG 622 58.121 1.103 23.30 2.586 1.00 36.40 ATOM 4780 C ARG 622 58.121 1.103 23.30 2.090 1.00 35.64 ATOM 4780 C ARG 622 58.121 1.103 23.30 2.090 1.00 35.04 ATOM 4780 C ARG 622 58.121 1.103 23.30 2.090 1.00 35.04 ATOM 4780 C ARG 622 58.128 11.103 22.499 1.00 35.04 ATOM 4780 C ARG 622 58.128 11.103 22.399 1.00 35.04 ATOM 4780 C ARG 622 58.128 11.103 61.00 25.00 ATOM 4780 C ARG 622 58.128 11.103 61.00 25.80 ATOM 4799 C ARG 622 58.128 11.103 61.00 25.00 ATOM 4799 C ARG 622 58.128 11.100 61.00 25.00 ATOM 4790 C ARG 622 58.60 61.00 680 10.00 35.04 ATOM 4790 C ARG 622 56.405 12.008 21.355 1.00 36.29 ATOM 4791 N A	ATOM 4752 N	62.465 8 645 27 335 1.00 32.13
ATOM 4755 CB ILE 620 61.046 10.999 26.708 1.00 32.75 ATOM 4756 CG2 ILE 620 60.440 12.129 27.421 1.00 32.75 ATOM 4757 CG1 ILE 620 659.002 12.339 26.986 1.00 33.55 ATOM 4758 CD1 ILE 620 659.002 12.339 26.986 1.00 33.55 ATOM 4758 CD1 ILE 620 60.486 11.913 28.933 1.00 30.71 ATOM 4760 0 ILE 620 60.969 11.086 25.206 1.00 30.11 ATOM 4761 N HIS 621 60.356 10.114 24.533 1.00 33.40 ATOM 4763 CA HIS 621 60.356 10.114 24.533 1.00 33.40 ATOM 4766 CD2 HIS 621 60.230 10.092 23.087 1.00 32.30 ATOM 4766 CD2 HIS 621 60.694 7.404 20.533 1.00 32.30 ATOM 4766 CD2 HIS 621 60.694 7.404 20.533 1.00 32.30 ATOM 4767 CD1 HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4769 CE1 HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4770 NE2 HIS 621 60.481 7.579 19.184 1.00 25.20 ATOM 4771 N ARG 622 58.128 11.363 22.499 1.00 35.40 ATOM 4772 C HIS 621 59.459 11.574 21.188 1.00 39.18 ATOM 4776 CA ARG 622 57.694 13.732 22.686 1.00 36.39 ATOM 4777 CB ARG 622 57.694 13.732 22.686 1.00 36.39 ATOM 4779 CD ARG 622 58.171 14.253 23.937 1.00 33.79 ATOM 4780 NE ARG 622 58.817 15.791 23.759 0.50 32.170 ATOM 4780 NE ARG 622 58.817 15.791 23.759 0.50 32.170 ATOM 4780 NE ARG 622 58.817 15.591 23.759 0.50 33.40 ATOM 4780 NE ARG 622 58.817 14.253 23.937 1.00 35.60 ATOM 4780 NE ARG 622 58.817 15.591 23.759 0.50 32.170 ATOM 4780 NE ARG 622 58.817 15.591 23.759 0.50 32.170 ATOM 4780 NE ARG 622 58.817 15.591 23.759 0.50 32.170 ATOM 4780 NE ARG 622 58.817 15.591 23.759 0.50 33.40 ATOM 4790 CD ARG 622 58.817 15.591 23.759 0.50 33.40 ATOM 4791 N ASP 623 56.606 10.938 20.668 1.00 35.68 ATOM 4793 CD ARG 622 58.605 10.938 20.668 1.00 35.04 ATOM 4794 CB ASP 623 56.607 12.808 20.99 1.00 35.08 ATOM 4799 CD ARG 622 56.005 12.008 21.355 1.00 36.23 ATOM 4799 CD ARG 622 56.607 12.808 20.99 1.00 35.04 ATOM 4799 CD ASP 623 56.607 12.808 20.99 1.00 37.70 ATOM 4800 N LEU 624 56.007 6.801 20.99 1.00 31.71 ATOM 4800 C LEU 624 56.009 6.801 20.99 1.00 31.71 ATOM 4808 CD LEU 624 56.009 6.801 20.99 1.00 35.74 ATOM 4808 CD LEU 624 56.009 6.801 20.99 1.00 27.00 ATOM 4809 C LEU 624 56.009 6.801 20.99	ATOM 4754 620	62.477 10.810 27.584 1.00 30.72
ATOM 4756 CG2 ILE 620	ATOM AZEC 020	61 046 26.960 1.00 32 70
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ATOM 4759 C ILE 620	ATOM 4750 CG1 ILE 620	60 496 1.00 38 39
ATOM 4760 0 ILE 620 60.969 11.086 25.206 1.00 30.11  ATOM 4761 N HIS 621 61.516 12.040 24 674 1.00 33.31  ATOM 4763 CA HIS 621 60.356 10.114 24.533 1.00 33.56  ATOM 4765 CG HIS 621 60.036 10.092 23.087 1.00 33.56  ATOM 4766 CD2 HIS 621 60.049 8.402 21.173 1.00 29.55  ATOM 4767 ND1 HIS 621 60.664 7.404 20.533 1.00 29.55  ATOM 4767 ND1 HIS 621 59.866 8.668 22.642 1.00 29.55  ATOM 4769 CEI HIS 621 59.866 9.73 20.187 1.00 25.20  ATOM 4770 NP2 HIS 621 59.462 9.173 20.187 1.00 25.81  ATOM 4770 NP2 HIS 621 59.246 11.103 22.499 1.00 25.81  ATOM 4773 U HIS 621 59.246 11.103 22.499 1.00 25.81  ATOM 4776 CA ARG 622 58.128 11.361 23.178 1.00 36.39  ATOM 4777 CB ARG 622 57.167 12.323 22.686 1.00 36.39  ATOM 4779 CD ARG 622 58.171 12.323 22.686 1.00 36.39  ATOM 4780 NE ARG 622 57.694 13.732 22.617 1.00 33.79  ATOM 4780 NE ARG 622 58.817 14.253 23.937 1.00 33.79  ATOM 4780 NE ARG 622 58.817 12.233 22.686 1.00 36.62  ATOM 4780 NE ARG 622 58.817 12.233 22.686 1.00 36.62  ATOM 4780 NE ARG 622 58.817 12.233 22.686 1.00 36.62  ATOM 4780 NE ARG 622 58.817 12.233 22.500 0.50 32.17  ATOM 4780 NE ARG 622 58.817 12.253 23.937 1.00 33.79  ATOM 4780 NE ARG 622 58.817 12.253 23.937 1.00 33.79  ATOM 4780 NE ARG 622 58.817 12.233 22.686 1.00 36.62  ATOM 4780 NE ARG 622 58.817 12.023 22.690 0.50 32.17  ATOM 4780 NE ARG 622 58.817 12.008 21.355 1.00 36.23  ATOM 4790 O ARG 622 58.837 15.591 23.759 0.50 33.44  ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23  ATOM 4790 O ARG 622 56.555 0.50 34.07  ATOM 4790 O ARG 623 56.664 8.645 12.003 2.82  ATOM 4790 O ARG 623 56.664 10.938 20.668 1.00 35.04  ATOM 4790 O ARG 623 56.564 12.008 21.355 1.00 35.64  ATOM 4790 O ARG 623 56.664 8.645 12.003 2.986  ATOM 4790 O ARG 623 56.664 8.645 12.000 29.10  ATOM 4800 N LEU 624 56.009 6.801 20.029 1.00 31.16  ATOM 4800 CD LEU 624 56.009 6.801 20.029 1.00 31.16  ATOM 4800 CD LEU 624 56.009 6.801 20.029 1.00 29.10  ATOM 4800 CD LEU 624 56.009 6.801 20.029 1.00 29.10  ATOM 4800 CD LEU 624 56.009 6.801 20.029 1.00 29.10  ATOM 4800 CD LEU 624 56.009 6.801 1.00 29.82	ATOM 1756 CDI ILE 620	59 994 73 28.933 1.00 30 71
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ATOM 4764 CB HIS 621 59.866 8.668 22.642 1.00 32.30 ATOM 4765 CG HIS 621 60.049 8.402 21.173 1.00 32.30 ATOM 4767 ND1 HIS 621 60.694 7.404 20.533 1.00 24.26 ATOM 4769 CEL HIS 621 59.866 8.668 22.642 1.00 29.55 ATOM 4769 CEL HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4770 NE2 HIS 621 59.462 9.173 20.187 1.00 25.81 ATOM 4770 NE2 HIS 621 59.462 9.173 20.187 1.00 25.81 ATOM 4771 NE2 HIS 621 59.462 9.173 20.187 1.00 25.81 ATOM 4773 U HIS 621 59.464 11.103 22.499 1.00 35.40 ATOM 4774 N ARG 621 59.464 11.103 22.499 1.00 35.40 ATOM 4776 CA ARG 622 59.459 11.574 21.388 1.00 39.18 ATOM 4776 CA ARG 622 57.117 12.323 22.6617 1.00 36.39 ATOM 4778 CG ARG 622 57.117 12.323 22.6617 1.00 36.39 ATOM 4779 CD ARG 622 58.837 15.591 23.759 0.50 32.17 ATOM 4780 NE ARG 622 59.315 16.101 25.032 0.50 32.17 ATOM 4780 NE ARG 622 59.315 16.101 25.032 0.50 32.17 ATOM 4780 NE ARG 622 60.803 16.268 26.769 0.50 33.44 ATOM 4791 CD ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4792 CD ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4793 CA ASP 623 56.105 12.008 21.355 1.00 35.68 ATOM 4793 CA ASP 623 56.574 11.032 18.221 1.00 35.68 ATOM 4795 CG ASP 623 56.574 11.032 18.221 1.00 35.68 ATOM 4796 OD ARG 622 56.405 12.008 21.355 1.00 35.04 ATOM 4797 OD ARG 622 56.405 12.008 21.355 1.00 35.04 ATOM 4798 C ASP 623 56.574 11.036 16.974 1.00 35.08 ATOM 4799 O ARG 623 56.574 11.032 18.221 1.00 35.08 ATOM 4799 OD ARG 623 56.606 10.938 20.668 1.00 35.04 ATOM 4796 OD1 ASP 623 56.574 11.032 18.221 1.00 36.23 ATOM 4797 OD2 ASP 623 56.574 11.032 18.221 1.00 33.79 ATOM 4798 C ASP 623 56.606 10.938 20.668 1.00 35.04 ATOM 4800 C LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.007 6.144 21.407 1.00 28.48 ATOM 4808 O LEU 624 56.007 6.801 20.029 1.00 31.71 ATOM 4808 O LEU 624 56.007 6.801 20.029 1.00 29.10 ATOM 4808 O LEU 624 56.007 6.801 20.029 1.00 29.10 ATOM 4808 O LEU 624 56.007 6.801 20.029 1.00 29.10 ATOM 4808 O LEU 624 56.007 6.801 18.081 1.00 29.82	W RIS 621	12.040 24 674 1 00 22
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ATOM 4766 CD2 HIS 621 60.694 7.404 20.533 1.00 24.26 ATOM 4769 CEI HIS 621 59.462 9.173 20.187 1.00 25.20 ATOM 4770 NE2 HIS 621 59.734 8.652 19.006 1.00 25.20 ATOM 4771 NE2 HIS 621 59.246 11.103 22.499 1.00 25.81 ATOM 4773 U HIS 621 59.246 11.103 22.499 1.00 25.81 ATOM 4773 U HIS 621 59.246 11.103 22.499 1.00 35.40 ATOM 4774 N ARG 622 58.128 11.363 23.178 1.00 36.39 ATOM 4776 CA ARG 622 57.171 12.323 22.686 1.00 36.39 ATOM 4777 CB ARG 622 57.694 13.732 22.517 1.00 36.40 ATOM 4779 CD ARG 622 58.171 14.253 23.937 1.00 33.79 ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17 ATOM 4782 CZ ARG 622 58.837 15.786 25.575 0.50 34.07 ATOM 4783 NH1 ARG 622 61.326 14.965 24.952 0.50 34.07 ATOM 4780 NH2 ARG 622 60.803 16.268 26.769 0.50 32.70 ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4791 N ASP 623 56.405 12.008 21.355 1.00 35.04 ATOM 4795 CG ASP 623 56.405 12.008 21.355 1.00 35.04 ATOM 4795 CG ASP 623 56.405 12.008 21.355 1.00 36.23 ATOM 4796 ODI ASP 623 56.574 11.352 18.221 1.00 35.84 ATOM 4795 CG ASP 623 56.405 12.008 21.355 1.00 36.23 ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 35.84 ATOM 4795 CG ASP 623 56.405 12.008 21.355 1.00 36.23 ATOM 4795 CG ASP 623 56.405 12.008 21.355 1.00 36.23 ATOM 4796 ODI ASP 623 56.574 11.352 18.221 1.00 35.84 ATOM 4796 ODI ASP 623 56.574 11.352 18.221 1.00 35.84 ATOM 4797 OD2 ASP 623 56.574 11.352 18.221 1.00 35.84 ATOM 4798 C ASP 623 56.574 11.352 18.221 1.00 35.84 ATOM 4799 O ASP 623 56.574 11.352 18.221 1.00 32.98 ATOM 4799 O ASP 623 56.574 11.352 18.221 1.00 32.98 ATOM 4799 O ASP 623 56.664 8.645 18.007 1.00 28.48 ATOM 4804 CG LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4808 O LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4808 O LEU 624 56.009 6.801 20.029 1.00 28.48 ATOM 4806 CD2 LEU 624 56.009 6.801 20.029 1.00 28.13 ATOM 4808 O LEU 624 56.009 6.801 20.029 1.00 28.13 ATOM 4808 O LEU 624 56.009 6.801 20.029 1.	Amout 4765 CG HIS 621	9.668 22 642
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ATOM 4770 NE2 HIS 621 59.734 8.652 19.006 1.00 25.20 ATOM 4772 C HIS 621 60.481 7.579 19.184 1.00 26.65 ATOM 4773 U HIS 621 59.246 11.103 22.499 1.00 25.581 ATOM 4774 N ARG 622 59.459 11.574 21.388 1.00 36.39 ATOM 4776 CA ARG 622 57.117 12.323 22.499 1.00 36.40 ATOM 4777 CB ARG 622 57.694 13.732 22.617 1.00 36.40 ATOM 4778 CG ARG 622 57.694 13.732 22.617 1.00 36.40 ATOM 4779 CD ARG 622 58.11 14.253 23.937 1.00 35.62 ATOM 4780 NE ARG 622 58.837 15.591 23.590 0.50 32.17 ATOM 4781 NAI ARG 622 58.837 15.591 23.590 0.50 32.17 ATOM 4782 CZ ARG 622 59.315 16.101 25.032 0.50 32.17 ATOM 4783 NH1 ARG 622 60.487 15.766 25.575 0.50 34.07 ATOM 4789 C ARG 622 60.803 16.268 26.769 0.50 33.44 ATOM 4790 O ARG 622 60.803 16.268 26.769 0.50 33.44 ATOM 4791 N ASP 623 56.405 12.008 21.355 1.00 36.23 ATOM 4794 CB ASP 623 56.6405 12.008 21.355 1.00 36.23 ATOM 4794 CB ASP 623 56.6128 10.538 19.436 1.00 35.68 ATOM 4795 CG ASP 623 56.574 11.036 16.974 1.00 35.68 ATOM 4796 OD1 ASP 623 56.574 11.036 16.974 1.00 46.29 ATOM 4799 O ASP 623 56.574 11.036 16.974 1.00 46.29 ATOM 4799 O ASP 623 56.627 11.082 15.851 1.00 30.990 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 30.990 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 30.990 ATOM 4799 O ASP 623 56.604 8.645 18.073 1.00 30.990 ATOM 4800 N LEU 624 56.009 6.801 20.029 1.00 31.16 ATOM 4803 CB LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4806 CD1 LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4807 C LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4808 O LEU 624 56.009 4.618 21.514 1.00 28.13 ATOM 4808 O LEU 624 56.009 4.618 21.514 1.00 28.13 ATOM 4808 O LEU 624 56.009 4.618 21.514 1.00 28.13 ATOM 4808 O LEU 624 56.009 4.618 21.514 1.00 28.13 ATOM 4808 O LEU 624 56.009 19.105 1.00 32.67	4767 1371 1370	7.404 20 535
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ATOM 4772 C HIS 621 59.246 11.103 22.499 1.00 35.40  ATOM 4774 N ARG 622 59.459 11.574 21.388 1.00 39.18  ATOM 4776 CA ARG 622 58.128 11.363 23.178 1.00 36.39  ATOM 4777 CB ARG 622 57.117 12.323 22.686 1.00 36.460  ATOM 4778 CG ARG 622 57.694 13.733 22.617 1.00 35.62  ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17  ATOM 4783 NH1 ARG 622 60.487 15.786 25.575 0.50 34.07  ATOM 4783 NH1 ARG 622 60.487 15.786 25.575 0.50 34.07  ATOM 4780 NE ARG 622 60.803 16.268 26.769 0.50 33.44  ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 35.04  ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.84  ATOM 4793 CA ASP 623 56.806 10.938 20.668 1.00 35.84  ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 35.68  ATOM 4796 OD1 ASP 623 56.277 11.082 15.851 1.00 36.23  ATOM 4799 O ASP 623 56.271 1.082 15.851 1.00 32.98  ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 30.90  ATOM 4799 O ASP 623 56.607 6.801 20.029 1.00 31.71  ATOM 4800 N LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.070 6.144 21.507 1.00 29.10  ATOM 4805 CD1 LEU 624 56.070 6.144 21.507 1.00 29.10  ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.82	4770 NE2 HTS CO.	59.734 8.652 12 005 4.00 25.20
ATOM 4773	A10M 4772 C HIS CO.	60.481 7.579 19.704
ATOM 4774 N ARG 622 58.128 11.574 21.388 1.06 39.18 ATOM 4776 CA ARG 622 57.117 12.323 22.686 1.00 36.39 ATOM 4777 CB ARG 622 57.694 13.732 22.686 1.00 36.40 ATOM 4780 NE ARG 622 58.8171 14.253 23.937 1.00 35.62 ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17 ATOM 4780 NE ARG 622 59.315 16.101 25.032 0.50 32.82 ATOM 4781 ARG 622 60.487 15.786 25.575 0.50 34.07 ATOM 4783 NH1 ARG 622 61.326 14.965 24.952 0.50 33.44 ATOM 4789 C ARG 622 66.803 16.268 26.769 0.50 32.70 ATOM 4790 O ARG 622 55.527 12.763 20.936 1.00 35.84 ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.84 ATOM 4794 CB ASP 623 56.128 10.538 19.436 1.00 35.84 ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 38.71 ATOM 4796 OD1 ASP 623 55.736 11.036 16.974 1.00 46.29 ATOM 4797 OD2 ASP 623 56.271 11.082 15.851 1.00 52.33 ATOM 4799 O ASP 623 56.271 11.082 15.851 1.00 50.45 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4799 O ASP 623 56.604 8.645 18.073 1.00 32.98 ATOM 4800 N LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4808 O LEU 624 56.070 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	4773 U HIS 631	59.246 11.103 22 402
ATOM 4776 CA ARG 622 57.117 12.323 22.686 1.00 36.39 ATOM 4777 CB ARG 622 57.694 13.732 22.617 1.00 36.40 ATOM 4779 CD ARG 622 58.171 14.253 23.937 1.00 36.40 ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17 ATOM 4781 NH1 ARG 622 59.315 16.101 25.032 0.50 32.82 ATOM 4786 NH2 ARG 622 60.487 15.766 25.575 0.50 34.07 ATOM 4789 C ARG 622 60.803 16.268 26.769 0.50 32.70 ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04 ATOM 4793 CA ASP 623 56.128 10.538 19.436 1.00 35.68 ATOM 4794 CB ASP 623 56.128 10.538 19.436 1.00 35.84 ATOM 4795 CG ASP 623 56.574 11.036 16.974 1.00 46.29 ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 32.33 ATOM 4798 C ASP 623 56.271 10.08 15.851 1.00 32.33 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4799 O ASP 623 56.604 8.645 18.073 1.00 30.90 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16 ATOM 4804 CG LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4804 CG LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4807 C LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4808 O LEU 624 56.099 4.618 21.514 1.00 28.13 ATOM 4807 C LEU 624 56.099 4.618 21.514 1.00 29.10 ATOM 4808 O LEU 624 56.099 4.618 21.514 1.00 29.10 ATOM 4808 O LEU 624 56.099 1.00 31.71 ATOM 4808 O LEU 624 56.099 1.00 32.98	ATOM 4774 N ADO	59.459 11.574 21 200 35.40
ATOM 4777 CB ARG 622 57.694 13.732 22.617 1.00 36.39  ATOM 4778 CG ARG 622 58.171 14.253 23.337 1.00 35.62  ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17  ATOM 4781 NH1 ARG 622 60.487 15.766 25.575 0.50 34.07  ATOM 4783 NH1 ARG 622 61.326 14.965 24.952 0.50 32.82  ATOM 4789 C ARG 622 60.803 16.268 26.769 0.50 32.70  ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23  ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.84  ATOM 4793 CA ASP 623 56.128 10.538 19.436 1.00 35.84  ATOM 4794 CB ASP 623 56.574 11.352 18.221 1.00 38.71  ATOM 4795 ODI ASP 623 56.574 11.036 16.974 1.00 46.29  ATOM 4797 OD2 ASP 623 56.271 1.082 15.851 1.00 52.33  ATOM 4799 O ASP 623 56.271 1.082 15.851 1.00 52.33  ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 30.90  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.71  ATOM 4803 CB LEU 624 56.009 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.009 6.801 20.029 1.00 31.71  ATOM 4807 C LEU 624 56.009 4.618 21.514 1.00 28.48  ATOM 4808 O LEU 624 56.072 4.283 22.997 1.00 29.10  ATOM 4808 O LEU 624 56.072 4.283 22.997 1.00 29.10  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 32.82	ATOM 4776 CA ADO	58.128 11.363 12 170
ATOM 4778 CG ARG 622 58.171 14.253 23.937 1.00 35.62 ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17 ATOM 4782 CZ ARG 622 59.315 16.101 25.032 0.50 32.82 ATOM 4783 NH1 ARG 622 60.487 15.786 25.575 0.50 34.07 ATOM 4786 NH2 ARG 622 60.803 16.268 26.769 0.50 32.47 ATOM 4789 C ARG 622 60.803 16.268 26.769 0.50 32.70 ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04 ATOM 4793 CA ASP 623 56.128 10.538 19.436 1.00 35.68 ATOM 4794 CB ASP 623 56.574 11.352 18.221 1.00 35.68 ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 35.68 ATOM 4796 OD1 ASP 623 56.574 11.036 16.974 1.00 46.29 ATOM 4798 C ASP 623 56.574 11.036 16.974 1.00 46.29 ATOM 4799 O ASP 623 56.574 11.036 16.974 1.00 35.04 ATOM 4799 O ASP 623 56.574 11.036 16.974 1.00 35.04 ATOM 4799 O ASP 623 56.574 11.036 16.974 1.00 32.98 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4798 C ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.71 ATOM 4804 CG LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4805 CD1 LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.82	ATOM 4777 CB NDG	57.117 12.323 22 525
ATOM 4780 NE ARG 622 58.837 15.591 23.759 0.50 32.17  ATOM 4782 CZ ARG 622 59.315 16.101 25.032 0.50 32.82  ATOM 4783 NH1 ARG 622 60.487 15.786 25.575 0.50 34.07  ATOM 4786 NH2 ARG 622 60.487 15.786 25.575 0.50 33.44  ATOM 4789 C ARG 622 60.803 16.268 26.769 0.50 32.70  ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23  ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04  ATOM 4793 CA ASP 623 56.128 10.538 19.436 1.00 35.68  ATOM 4794 CB ASP 623 56.574 11.352 18.221 1.00 35.68  ATOM 4796 OD1 ASP 623 56.574 11.352 18.221 1.00 35.68  ATOM 4797 OD2 ASP 623 56.574 11.036 16.974 1.00 46.29  ATOM 4798 C ASP 623 56.277 11.082 15.851 1.00 52.33  ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98  ATOM 4799 C ASP 623 56.664 8.645 18.073 1.00 30.90  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.71  ATOM 4804 CG LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4805 CD1 LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4806 CD2 LEU 624 56.049 4.618 21.514 1.00 28.48  ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.82	ATOM 4778 CG ARC	57.694 13.732 22 620
ATOM 4780 NE ARG 622 59.315 16.101 25.032 0.50 32.17 ATOM 4783 NH1 ARG 622 60.487 15.786 25.575 0.50 34.07 ATOM 4788 NH2 ARG 622 61.326 14.965 24.952 0.50 33.44 ATOM 4789 C ARG 622 60.803 16.268 21.355 1.00 36.23 ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04 ATOM 4793 CA ASP 623 56.128 10.538 19.436 1.00 35.84 ATOM 4794 CB ASP 623 56.574 11.352 18.221 1.00 38.71 ATOM 4795 CG ASP 623 55.573 11.082 15.851 1.00 46.29 ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33 ATOM 4798 C ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.71 ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4804 CG LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4805 CD1 LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4807 C LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 29.82	ATOM 4779 CD ARG	58.171 14.253 23 227 1.00 35.62
ATOM 4782 CZ ARG 622 59,315 16.101 25.032 0.50 32.82  ATOM 4783 NH1 ARG 622 60.487 15.786 25.575 0.50 34.07  ATOM 4786 NH2 ARG 622 61.326 14.965 24.952 0.50 33.44  ATOM 4789 C ARG 622 56.405 12.008 21.355 1.00 36.23  ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04  ATOM 4793 CA ASP 623 56.806 10.938 20.668 1.00 35.84  ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 35.68  ATOM 4796 OD1 ASP 623 55.736 11.036 16.974 1.00 46.29  ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33  ATOM 4799 C ASP 623 56.271 9.052 19.162 1.00 32.98  ATOM 4799 C ASP 623 56.664 8.645 18.073 1.00 30.90  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16  ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.009 6.801 20.029 1.00 31.71  ATOM 4805 CD1 LEU 624 56.009 6.801 20.029 1.00 31.71  ATOM 4806 CD2 LEU 624 56.009 6.801 20.029 1.00 31.71  ATOM 4807 C LEU 624 56.070 6.144 21.407 1.00 28.48  ATOM 4808 O LEU 624 56.072 4.283 22.987 1.00 27.00  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4780 NF ARG	58.837 15 501 1.00 33.79
ATOM 4783 NH1 ARG 622 61.326 14.965 24.952 0.50 34.07 ATOM 4786 NH2 ARG 622 60.803 16.268 26.769 0.50 33.44 ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04 ATOM 4794 CB ASP 623 56.574 11.352 18.221 1.00 35.68 ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 35.68 ATOM 4796 OD1 ASP 623 55.576 11.036 16.974 1.00 35.68 ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33 ATOM 4798 C ASP 623 56.277 11.082 15.851 1.00 52.33 ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98 ATOM 4790 O ASP 623 56.664 8.645 18.073 1.00 30.90 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16 ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4804 CG LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4805 CD1 LEU 624 56.009 6.801 20.029 1.00 31.71 ATOM 4806 CD2 LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 27.00 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4782 C7 ADO	59,315 16.101 25 022
ATOM 4786 NH2 ARG 622 61.326 14.965 24.952 0.50 33.44  ATOM 4789 C ARG 622 56.405 12.008 21.355 1.00 36.23  ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04  ATOM 4793 CA ASP 623 56.686 10.938 20.668 1.00 35.84  ATOM 4794 CB ASP 623 56.574 11.352 18.221 1.00 35.68  ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 38.71  ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 46.29  ATOM 4798 C ASP 623 56.277 11.082 15.851 1.00 52.33  ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98  ATOM 4709 O ASP 623 56.664 8.645 18.073 1.00 30.90  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16  ATOM 4804 CG LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48  ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13  ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4808 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4783 NW3 ADG	60.487 15.786 25 525
ATOM 4789 C ARG 622 56.405 12.008 21.355 1.00 36.23 ATOM 4791 N ASP 623 55.527 12.763 20.936 1.00 35.04 ATOM 4793 CA ASP 623 56.806 10.938 20.668 1.00 35.84 ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 38.71 ATOM 4796 OD1 ASP 623 55.576 11.036 16.974 1.00 46.29 ATOM 4797 OD2 ASP 623 55.277 11.082 15.851 1.00 52.33 ATOM 4798 C ASP 623 56.277 11.082 15.851 1.00 52.33 ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16 ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4805 CD1 LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4806 CD2 LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4786 MU2 NDG 622	61.326 14 965 25.575 0.50 34.07
ATOM 4790 O ARG 622 56.405 12.008 21.355 1.00 36.23  ATOM 4791 N ASP 623 56.806 10.938 20.668 1.00 35.04  ATOM 4794 CB ASP 623 56.128 10.538 19.436 1.00 35.68  ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 38.71  ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 46.29  ATOM 4799 O ASP 623 56.277 11.082 15.851 1.00 52.33  ATOM 4799 O ASP 623 56.271 10.082 15.851 1.00 50.45  ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 30.90  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16  ATOM 4803 CB LEU 624 56.070 6.144 21.407 1.00 28.48  ATOM 4806 CD2 LEU 624 56.070 6.144 21.407 1.00 28.13  ATOM 4806 CD2 LEU 624 56.070 6.144 21.407 1.00 28.13  ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4789 C ARG 622	60,803 16 360 24.952 0.50 33.44
ATOM 4791 N ASP 623 55.527 12.763 20.936 1.00 36.23  ATOM 4793 CA ASP 623 56.806 10.938 20.668 1.00 35.04  ATOM 4794 CB ASP 623 56.128 10.538 19.436 1.00 35.84  ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 38.71  ATOM 4796 OD1 ASP 623 55.736 11.036 16.974 1.00 46.29  ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33  ATOM 4798 C ASP 623 54.535 10.715 17.119 1.00 50.45  ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16  ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4805 CD1 LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4806 CD2 LEU 624 56.099 4.618 21.514 1.00 28.13  ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4790 0 ARG 622	56.405 12 000 0.50 32.70
ATOM 4793 CA ASP 623 56.806 10.938 20.668 1.00 35.04 ATOM 4794 CB ASP 623 56.128 10.538 19.436 1.00 35.84 ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 38.71 ATOM 4796 OD1 ASP 623 55.736 11.036 16.974 1.00 46.29 ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33 ATOM 4798 C ASP 623 54.535 10.715 17.119 1.00 50.45 ATOM 4799 O ASP 623 56.664 8.645 18.073 1.00 32.98 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16 ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4804 CG LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13 ATOM 4806 CD2 LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4807 C LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4808 O LEU 624 53.763 6.608 19.508 1.00 35.74 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4791 N 300	55.527 12 762 21.355 1.00 36.23
ATOM 4794 CB ASP 623 56.128 10.538 19.436 1.00 35.84  ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 38.71  ATOM 4796 OD1 ASP 623 55.736 11.036 16.974 1.00 46.29  ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33  ATOM 4798 C ASP 623 54.535 10.715 17.119 1.00 50.45  ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 30.90  ATOM 4802 CA LEU 624 56.015 8.244 20.179 1.00 31.16  ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48  ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13  ATOM 4806 CD2 LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4807 C LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4808 O LEU 624 53.763 6.608 19.508 1.00 35.74  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4793 CD 757	56.806 10 939 20.936 1.00 35.04
ATOM 4795 CG ASP 623 56.574 11.352 18.221 1.00 35.68 ATOM 4796 OD1 ASP 623 55.736 11.036 16.974 1.00 46.29 ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33 ATOM 4798 C ASP 623 54.535 10.715 17.119 1.00 50.45 ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 30.90 ATOM 4802 CA LEU 624 56.099 6.801 20.029 1.00 31.16 ATOM 4803 CB LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13 ATOM 4806 CD2 LEU 624 56.070 4.283 22.987 1.00 29.10 ATOM 4807 C LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4808 O LEU 624 53.763 6.608 19.508 1.00 35.74 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4794 CD 300	56.128 10.530 20.668 1.00 35.84
ATOM 4796 OD1 ASP 623 55.736 11.036 16.974 1.00 38.71 ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 52.33 ATOM 4798 C ASP 623 54.535 10.715 17.119 1.00 50.45 ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16 ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13 ATOM 4806 CD2 LEU 624 56.070 4.618 21.514 1.00 28.13 ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4795 CC 100	56.574 11 353 1.00 35.68
ATOM 4797 OD2 ASP 623 56.277 11.082 15.851 1.00 46.29  ATOM 4798 C ASP 623 54.535 10.715 17.119 1.00 50.45  ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16  ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48  ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13  ATOM 4806 CD2 LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4706	55.736 11.036 18.221 1.00 38.71
ATOM 4798 C ASP 623 54.535 10.715 17.119 1.00 52.33 ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98 ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16 ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71 ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13 ATOM 4806 CD2 LEU 624 57.225 3.975 20.799 1.00 27.00 ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 623	56.277 13 002 15 974 1.00 46.29
ATOM 4799 O ASP 623 56.271 9.052 19.162 1.00 32.98  ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 31.16  ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48  ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13  ATOM 4806 CD2 LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4700 0	54.535 10.715
ATOM 4800 N LEU 624 56.015 8.244 20.179 1.00 32.98 ATOM 4802 CA LEU 624 56.099 6.801 20.029 1.00 31.16 ATOM 4803 CB LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13 ATOM 4806 CD2 LEU 624 56.072 4.283 22.987 1.00 27.00 ATOM 4807 C LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4799 623	56 221 -17.119 1.00 50 45
ATOM 4802 CA LEU 624 56.015 8.244 20.179 1.00 30.90  ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.71  ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48  ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13  ATOM 4806 CD2 LEU 624 56.072 4.283 22.987 1.00 27.00  ATOM 4807 C LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4808 O LEU 624 53.763 6.608 19.508 1.00 35.74  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM ASP 623	56 664 19.162 1.00 32 98
ATOM 4803 CB LEU 624 56.099 6.801 20.029 1.00 31.16 ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13 ATOM 4806 CD2 LEU 624 57.225 3.975 20.799 1.00 27.00 ATOM 4807 C LEU 624 54.917 6.320 19.185 1.00 29.10 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 4800 - LEU 624	56 035 18.073 1.00 30 90
ATOM 4804 CG LEU 624 56.070 6.144 21.407 1.00 28.48 ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.13 ATOM 4806 CD2 LEU 624 57.225 3.975 20.799 1.00 27.00 ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM 1803	56 000 3.244 20.179 1.00 31 16
ATOM 4805 CD1 LEU 624 56.049 4.618 21.514 1.00 28.48  ATOM 4806 CD2 LEU 624 57.225 3.975 20.799 1.00 27.00  ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10  ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67  ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATOM LEU 624	56 070 20.001 20.029 1.00 31 71
ATOM 4806 CD2 LEU 624 57.225 3.975 20.799 1.00 27.00 ATOM 4807 C LEU 624 56.072 4.283 22.987 1.00 29.10 ATOM 4808 O LEU 624 53.763 6.608 19.508 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	ATCM 4804 CG LEU 624	56 040 21.407 1.00 28 40
ATOM 4806 CD2 LEU 624 56.072 4.283 22.987 1.00 27.00 ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	1701 4805 CD1 LEU 624	57 225 41.514 1.00 28 12
ATOM 4808 O LEU 624 54.917 6.320 19.185 1.00 29.10 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	1001 4806 CD2 LEU 624	56 072 3.975 20.799 1.00 27 00
ATOM 4808 O LEU 624 53.763 6.608 19.185 1.00 32.67 ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	4807 C LEU 524	36.072 4.283 22.987 1 00 20 20
ATOM 4809 N ALA 625 55.214 5.640 18.081 1.00 29.82	AMON 4808 O LEU 624	6.320 19.185 1 00 32 55
5.640 18.081 1.00 29.82	ATOM 4800 N	55.763 6.608 19.508 1.00 35.74
00 29.82		33.214 6 646
	SSSD/55145, v01	23.82

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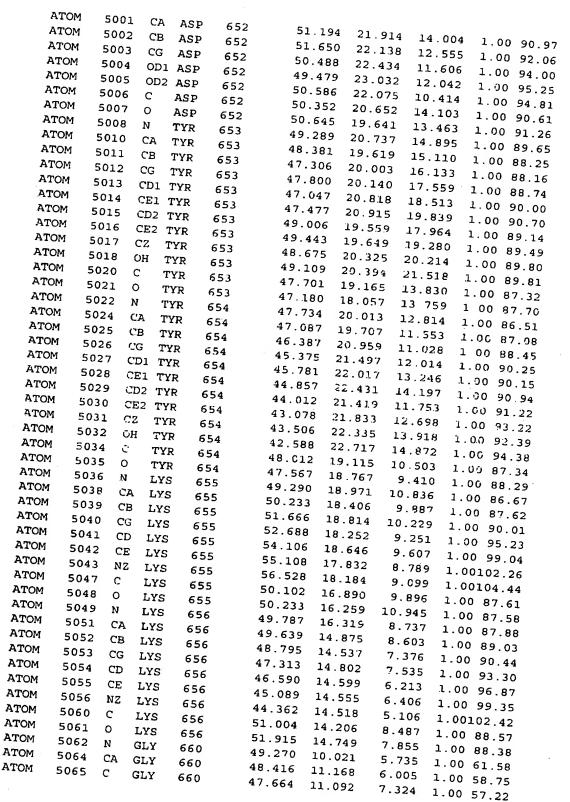
ATOM	4811	CA	ALA	625	54.194	5.106	17.181	1.00	28.29
MOTA	4812	CB	ALA	625	53.682	6.182	16.245	1.00	26.72
ATOM	4813	C	ALA	625	54.895	4.031	16.395	1.00	28.40
ATOM	4814	0	ALA	625	56.118	4.028	16.343	1.00	32.12
ATOM	4815	N	ALA	626	54.131	3.135	15.770	1.00	28.55
MOTA	4817	CA	ALA	626	54.687	2.028	14.979	1.00	26.25
ATOM	4818	CB	ALA	626	53.577	1.169	14.365	1.00	23.54
MOTA	4819	С	ALA	626	55.569	2.573	13.892	1.00	23.68
ATOM	4820	0	ALA	626	56.544	1.944	13.519	1.00	26.07
ATOM	4821	N	ARG	627	55.208	3.744	13.378	1.00	23.80
MOTA	4823	CA	ARG	627	55.980	4.413	12.338	1.00	26.57
ATOM	4824	CB	ARG	627	55.289	5.728	11.914	1.00	25.91
MOTA	4825	CG	ARG	627	54.991	6.692	13.055	1.00	27.60
MOTA	4826	CD	ARG	627	54.711	8.130	12.584	1.00	33.01
MOTA	4827	NE	ARG	627	54.260	8.978	13.691	1.00	34.18
ATOM	4829	CZ	ARG	627	52.997	9.067	14.091	1.00	35.88
ATOM	4830			627	52.056	8.380	13.460	1.00	38.89
ATOM	4833	NH2	ARG	627	52.689	9.748	15.183		36.43
ATOM	4836	С	ARG	627	57.439	4.686	12.785		29.03
ATOM	4837	0	ARG	627	58.362	4.636	11.972		29.24
ATOM	4838	N	ASN	628	57.634	4.938	14.087		29.51
ATOM	4840	CA	ASN	628	58.954	5.234.	14.645		26.41
ATOM	4841	CB	ASN	628	58.864	6.359	15.676		25.32
ATOM	4842	CG	ASN	628	58.539	7.687	15.035		28.11
ATOM	4843	ODI		628	59.079	8.028	13.999		32.09
ATOM	4844	ND2	ASN	628	57.639	8.426	15.628		27.88
MOTA	4847	C C	ASN	628	59.684	4.039	15.225		25.77
ATOM	4848	O N	ASN	628	60.641	4.188	16.001		24.77
ATOM ATOM	4849 4851	N CA	VAL VAL	629 629	59.209 59.828	2.853	14.874		26.63
ATOM	4852	CB	VAL	629	58.812	1.610 0.693	15.315 16.007	1.00	25.34
ATOM	4853	CG1		629	59.492	-0.604	16.412		22.96
ATOM	4854	CG2	VAL	629	. 58.205	1.398	17.207		16.65
ATOM	4855	C	VAL	629	60.266	0.962	14.007		26.79
ATOM	4856	Ö	VAL	629	59.454	0.839	13.087		28.60
ATOM	4857	N	LEU	630	61.542	0.603	13.904	1.00	
ATOM	4859	CA	LEU	630	62.062	-0.021	12.685	1.00	
ATOM	4860	CB	LEU	630	63.297	0.733	12.210	1.00	
ATOM	4861	CG	LEU	630	63.044	2.242	12.111		
ATOM	4862	CD1	LEU	630	64.345	2.944	11.972	1.00	
ATOM	4863		LEU	630	62.111	2.603	10.965	1.00	
ATOM	4864	C	LEU	630	62.367	-1.492	12.961	1.00	
ATOM	4865	0	LEU	630	62.629	-1.852	14.101	1.00	
ATOM	4866	N	VAL	631	62.246	-2.346	11.946	1.00	
ATOM	4868	CA	VAL	631	62.468	-3.790	12.098	1.00	
ATOM	4869	CB	VAL	631	61.194	-4.607	11.659	1.00	
ATOM	4870		VAL	631	61.346	-6.085	12.026	1.00	
ATOM	4871		VAL	631	59.937	-4.030	12.290	1.00	
MOTA	4872	С	VAL	631	63.697	-4.286	11.305	1.00	
ATOM	4873	0	VAL	631	63.849	-3.999	10.097	1.00	
MOTA	4874	N	THR	632	64.551	-5.052	11.979	1.00	
MOTA	4876	CA	THR	632	65.770	-5.574	11.365	1.00	

				*
	TOM 48	77 CB	THR 63	) n
	TOM 48	78 OG1	·	- 5.836 12 416 3 6-
	TOM 48	80 CG2		66.423 -6.908 13 272 1 00
	TOM 48			67.069 -4.582 13 238 1 23
	TOM 48		<b>5</b> 111-	65.526 -6.854 10.503 1.00 40.22
A:	TOM 488		~~	64.471 -7.457 10 244 3 39.17
	rom 488		~	3 66.496 -7.259 9.766 1.00 41.26
PΑ	OM 488			66.397 -9.403
PΑ	OM 488	7	a	67.677 -0 713 - 1.00 42.62
AT	OM 488	^	GLU 63	67.610 -9.004
AT			GLU 633	66.825 0 50.
AT	OM 489	^	~*	66.390 0 444
AT			GLU 633	66.651 -10 536 1.00 62.64
ATO		` - `	GLU 633	66.097 733
ATO			ELU 633	65.578 -10.704
ATC			ISP 634	66.415 -9.665 9.288 1.00 42.77
ATC			SP 634	66.167 -10 704 11.082 1.00 43.14
ATO		7	SP 634	67 361 45 11.978 1.00 44.01
ATO		7	SP 634	59 636 12.914 1.00 49 37
ATO		OD1 A	SP 634	68 692 12.166 1.00 54.70
ATO	*000	OD2 A		69 602 11.595 1.00 55 43
ATO		C As		64 035 12.167 1.00 56 17
ATO		O AS	SP 634	64 754 12.801 1.00 43.95
ATON		N AS	SN 635	64.075 13.864 1.00 45.92
ATOM		CA AS	N 635	62 822 2.316 1.00 44.71
ATOM	-505	CB AS	N 635	61 854 +2 12.980 1.00 43.07
ATOM		CG AS		61 606 10.404 13.018 1.00 45.50
ATOM		OD1 AS	N 635	60 907 11.653 1.00 45 43
ATOM		ND2 ASI	N 635	52 174 10.788 1.00 49 56
ATOM		C ASI	N 635	62 027
ATOM		O ASI	V 635	62 050 - 14.380 1.00 41.64
ATOM		N VAI		63 004 - 15.221 1.00 41.69
ATOM	4915	CA AVI		64 177 14.627 1.00 41 17
ATOM	4916	CB VAL	636	65 602 - 15.922 1.00 39.01
ATOM	4917	CG1 VAL	636	65 882 7.002 16.259 1.00 40.66
ATOM	4918	CG2 VAL	636	66 355 17.560 1.00 35.04
ATOM		C VAL		63 544 - 16.367 1.00 41 69
ATOM		O VAL	636	63 917 15.925 1.00 36 77
ATOM		N MET	637	62 606 15,045 1.00 38.35
ATOM		CA MET	637	62 040 3.318 16.908 1.00 35 71
	4924	CB MET	637	1,7,031 1 00 22 c-
ATOM	4925 (	G MET	637	50 777
ATOM		D MET	637	1/.371 1 00 41 2.
ATOM		E MET	637	15,695 1 00 42 24
ATOM	4928	MET	637	14.976 1 00 30 37
ATOM	4929 C	MET	637	3.209 17.668 1 00 32 62
ATOM	4930 N		638	63.524 -3.436 18.765 1.00 30 56
ATOM	4932 C		638	03.1/3 -2.070 17.008 1 00 33 05
ATOM	4933 C		638	04.073 -1.027 17.492 1 00 30 37
ATOM	4934 C		638	65.351 -1.022 16.654 1 00 37 75
ATOM	4935 CI		638	00.245 -2.211 16.896 1 00 35 0
ATOM	4936 CI		638	67.429 -2.170 15.976 1 00 24.50
ATOM	4937 NZ		638	68.443 ~3.187 16.390 1 00 33 05
			338	69.121 -2.803 17.651 1.00 24.79
				4.00 24.79



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ATOM	4941	С	LYS	638	63.443	0.364	17.446	1.00 28.00
ATOM	4942	0	LYS	638	62.977	0.799	16.391	1.00 25.60
ATOM	4943	N	ILE	639	63.410	1.032	18.601	1.00 25.32
ATOM	4945	CA	ILE	639	62.857	2.379	18.721	1.00 25.91
MOTA	4946	CB	ILE	639	62.800	2.875	20.201	1.00 25.56
MOTA	4947	CG2	ILE	639	62.074	4.208	20.279	1.00 22.82
ATOM	4948	CG1	ILE	639	62.142	1.835	21.118	1.00 28.00
ATOM	4949	CD1	ILE	639	60.634	1.748	21.003	1.00 33.25
ATOM	4950	C	ILE	639	63.739	3.363	17.955	1.00 26.87
MOTA	4951	0	ILE	639	64.968	3.381	18.125	1.00 24.13
MOTA	4952	N	ALA	640	63.108	4.170	17.108	1.00 26.74
ATOM	4954	CA	ALA	640	63.825	5.176	16.339	1.00 30.62
ATOM	4955	CB	ALA	640	63.624	4.939	14.851	1.00 30.31
ATOM	4956	C	ALA	640	63.338	6.572	16.739	1.00 32.53
MOTA	4957	0	ALA	640	62.289	6.706	17.371	1.00 33.83
MOTA	4958	N	ASP	641	64.082	7.605	16.351	1.00 33.05
MOTA	4960	CA	ASP	641	63.749	9.010	16.656	1.00 37.66
ATOM	4961	CB	ASP	641	62.539	9.489	15.840	1.00 42.62
ATOM	4962	CG	ASP	641	62.928	10.026	14.471	1.00 50.92
ATOM	4963	OD1	ASP	641	64.092	9.833	14.021	1.00 59.21
ATOM	4964	QD2	ASP	641	62.063	10.652	13.823	1.00 54.05
MOTA	4965	С	ASP	641	63.545	9.367	18.125	1.00 37.85
ATOM	4966	0	ASP	641	62.805	10.294	18.448	1.00 39.10
ATOM	4967	N	PHE	642	64.204	8.635	19.016	1.00 37.47
ATOM	4969	CA	PHE	642	64.099	8.874	20.456	1.00 36.47
MOTA	4970	CB	PHE	642	64.403	7.581	21.226	1.00 32.22
ATOM	4971	CG	PHE	642	65.786	7.013	20.964	1.00 30.65
ATOM	4972	CD1	PHE	642	66.906	7.537	21.607	1.00 32.45
ATOM	4973	CD2	PHE	642	65. <b>96</b> 9	5.981	20.054	1.00 28.53
ATOM	4974	CE1	PHE	642	68.180	7.050	21.342	1.00 30.88
ATOM	4975	CE2	PHE	642	67.234	5.494	19.789	1.00 27.74
ATOM	4976	CZ	PHE	642	68.344	6.027	20 431	1.00 29.64
MOTA	4977	С	PHE	642	65.050	10.001	20.997	1.00 39.69
MOTA	4978	0	PHE	642	64.967	10.469	22.047	1.00 38.22
ATOM	4979	N	GLY	643	65.966	10.400	20.015	1.00 41.08
ATOM	4981	CA	GLY	643	66.925	11.447	20.324	1.00 40.65
ATOM	4982	C	GLY	643	66.694	12.747	19.571	1.00 43.53
ATOM	4983	0	GLY	643	67.500	13.666	19.688	1.00 41.10
ATOM	4984	N	LEU	644	65.617	12.825	18.786	1.00 48.35
ATOM	4986	CA	LEU	644	65.306	14.034	18.019	1.00 51.11
ATOM	4987	CB	LEU	644	63.962	13.907	17.314	1.00 50.28
ATOM	4988	CG	LEU	644	63.900	13.059	16.057	1.00 54.03
ATOM	4989		LEU	644	62.541	13.278	15.413	1.00 57.34
ATOM	4990		LEU	644	65.006	13.467	15.105	1.00 56.95
MOTA	4991	C	LEU	644	65.248	15.257	18.894	1.00 52.68
ATOM	4992	0	LEU	644	64.850	15.175	20.053	1.00 54.95
ATOM	4993	N	ALA	645	65629	16.399	18.332	1.00 54.61
ATOM	4995	CA	ALA	645	65.610	17.656	19.073	1.00 54.60
ATOM	4996	CB	ALA	645	66.495	18.684	18.382	1.00 53.32
ATOM	4997	C	ALA	645	64.178	18.185	19.215	1.00 54.09
ATOM	4998	0	ALA	645	63.716	18.488	20.322	1.00 53.14
ATOM	4999	N	ASP	652	52.340	21.795	14.895	1.00 91.33



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MOTA	5066	0	GLY	660	46.555	11.624	7.437	1.00 58.01
ATOM	5067	N	ARG	661	48.231	10.374	8.293	1.00 55.37
ATOM	5069	CA	ARG	661	47.631	10.247	9.622	1.00 51.19
ATOM	5070	CB	ARG	661	48.095	8.965	10.337	1.00 51.89
MOTA	5071	CG	ARG	661	47.756	7.663	9.612	1.00 51.56
MOTA	5072	CD	ARG	661	48.057	6.443	10.484	1.00 50.77
MOTA	5073	NE	ARG	661	47.834	5.181	9.772	1.00 50.04
MOTA	5075	CZ	ARG	661	48.015	3.974	10.307	1.00 48.12
ATOM	5076	NH1	ARG	661	48.421	3.855	11.569	1.00 43.28
ATOM	5079	NH2		661	47.788	2.882	9.578	1.00 43.69
ATOM	5082	С	AR.G	661	48.041	11.463	10.446	1.00 46.22
ATOM	5083	O	ARG	661	48.998	12.162	10.097	1.00 44.78
ATOM	5084	N	LEU	662	47.328	11.703	11.542	1.00 41.80
. ATOM	5086	CA	LEU	662	47.621	12.837	12.419	1.00 36.78
MOTA	5087	CB	LEU	662	46.342	13.596	12.758	1.00 33.05
ATOM	5088	C.C.	LEU	662	45.642	14.279	11.585	1.00 28.24
ATOM	5089	CD1	LEU	662	44.198	147.611	11.935	1.00 24.66
ATOM	5090	CD2	LEU	662	46.429	15.511	11.217	1.00 28.35
ATOM	5091	C	LEU	662	48.278	12.328	13.695	1.00 36.10
MOTA	5092	C	LEU	662	47.695	11.521	14.431	1.00 34.46
MOTA	5093	N	PRO	663	49.526	12.751	13.945	1.00 35.83
MOTA	5094	CD	PRO	663	50.360	13.537	13.022	1.00 37.72
ATOM	5095	CA	PRO	663	50.310	12.365	15.119	1.00 35.68
MOTA	5096	CB	PRO	663	51.611	13.130	14.914	1.00 35.23
ATOM	5097	CG	PRO	563	51.756	13.134	13.437	1.00 36.10
MOTA	5098	C	PRO	663	49.660		16.453	1.00 35.87
ATOM	5099	0	PRO	663	49.958	12.069	17.469	1.00 39.86
ATOM	5100	N	VAL	664	48.787	13.705	16.466	1.00 33.54
ATOM	5102	CA	VAL	664	48.109	14.076	17.699	1.00 31.24
ATOM	5103	CB	VAL	664	47.196	15.321	17.520	1.00 30.45
ATOM	5104	CG1	VAL	664	48.025	16.480	17.051	1.00 32.54
ATOM	5105	CG2	VAL	664	46.093	15.062	16.523	1.00 34.77
ATOM	5106	C	VAL	664	47.301	12.895	18.233	1.00 31.33
ATOM	5107	0	VAL	664	47.095	12.782	19.438	1.00 32.66
ATOM	5108	N	LYS	665	46.940	11.968	17.345	1.00 30.44
ATOM	5110	CA	LYS	665	46.153	10.795	17.719	1.00 28.43
ATOM	5111	CB	LYS	665	45.596	10.133	16.466	1.00 24.82
ATOM	5112	CG	LYS	665	44.700	11.086	15.687	1.00 27.50
ATOM	5113	CD	LYS	665	44.096	10.466	14.442	1.00 26.62
ATOM	5114	CE	LYS	665	42.967	11.326	13.909	1.00 21.64
ATOM	5115	NZ	LYS	665	42.479	10.850	12.584	1.00 25.29
ATOM	5119	C	LYS	665	46.889	9.794	18.615	1.00 29.56
ATOM	5120	0	LYS	665	46.295	8.836	19.095	1.00 29.57
ATOM	5121	N	TRP	666	48.183	10.020	18.826	1.00 30.12
ATOM	5123	CA	TRP	666	48.987	9.174	19.704	1.00 31.39
MOTA	5124	CB	TRP	666	50.329	8.845	19.059	1.00 30.40
MOTA	5125	CG	TRP	666	50.263	7.700	18.106	1.00 30.79
MOTA	5126	CD2		666	49.701	7.719	16.785	1.00 30.22
MOTA	5127	CE2	TRP	666	49.891	6.430	16.245	1.00 28.24
ATOM	5128	CE3	TRP	666	49.067	8.702	16.012	1.00 30.60
ATOM	5129	CD1		666	50.743	6.435	18.307	1.00 28.07
ATOM	5130	NE1	TRP	666	50.522	5.670	17.187	1.00 29.15

λ,	ТОМ	<b>5 7 7 0</b>			
		5132	CZ2		
		5133		TRP 666	48.640 9 224 1.00 29.38
		5134	CH2	TRP 666	48.845 7.005 14.726 1.00 31.27
	1014	5135	С	TRP 666	49 242 2 202 14.213 1.00 31.33
		5136	0	TRP 666	49 501 9.902 21.026 1.00 33.92
		5137	N	MET 667	49 020 22.040 1.00 35.23
AT		139	CA	MET 667	49 350 11.214 21.007 1.00 35.72
AT		140	CB I	MET 667	12.065 22.159 1.00 36.43
AT		141	CG I	MET 667	13.329 21.751 1 00 37 70
AT		142	SD N	1ET 667	14.194 21.574 1 00 40 10
ATO		143		1ET 667	13.906 21.096 1 00 46 03
ATO		144	_	ET 667	50.914 15.810 19.386 1 00 40 40
ATC		145		ET 667	48.389 11.839 23 370 1 00
ATC	)M 51	146		LA 668	47.186 11.646 23 273 1 00 25
ATO	M 51	148		LA 668	49.027 11.885 24 542 1 00 5
ATO					48.345 11.733 25 815 1 00 -
ATO.					49.351 11.537 26 929 1 00
ATO			_	· ·	47.603 13.038 26.014 1.00 37.61
ATO			N PI		48.059 14.000
ATO					46.474 13.001 26 731 1.00 39.40
ATON	1 51	_			45 842 13 000
ATOM					45.677 14 204 2.77
ATOM				-	44.609 13 600 1-100 43.91
ATOM	519				44 421 12 270 1.00 44.49
ATOM					46.476 15 373 27.439 1.00 43.59
ATOM					46.394 15 405 1.00 44.89
ATOM			_	•	47.266 15 107 27.073 1.00 45.48
ATOM				٠.٠	48,050 16 350 75 1.00 43.39
ATOM		-			48.739 15 645
ATOM	516				49.864 14.646 1.00 43.31
ATOM	516			-	49 408 12 02:
ATOM	516		E1 GLU		50.225 12 222
ATOM	5166		E2 GLU	-	48.235 12 033
ATOM	516	-	GLU	•	49.090 76.700
ATOM	5168		GLU	670	49.362 17.003
ATOM	5169		ALA	671	49.677 16.000 44.68
ATOM	5171			671	50.686 16.532
	5172		ALA	671	51 413 - 26.513 1.00 44.44
ATOM	5173		ALA	671	50.045 13.347 25.841 1.00 40.17
ATOM	5174	0	ALA	671	50.550 17.410 25.465 1.00 46.49
ATOM	5175	N	LEU	672	48 903 16 97 25.148 1.00 45.70
ATOM	5177	CA	LEU	672	48 163 10.970 24.952 1.00 50.30
ATOM	5178	CB	LEU	672	47 000 23.925 1.00 52.07
ATOM	5179	CG	LEU	672	46 300 == 23.335 1.00 54.41
ATOM	5180	CD1	LEU	672	17.103 22.005 1.00 57 12
ATOM	5181	CD2	LEU	672	17.316 20.912 7 00 57 65
MOTA	5182	С	LEU	672	13.951 21.640 1.00 56 14
ATOM	5183	0	LEU	672	47.535 18.964 24.512 1 00 52 42
ATOM	5184	N	PHE	673	47.683 20.058 23.969 1 00 52 71
MOTA	5186	CA	PHE	673 673	46.863 18.803 25.645 1 00 52 74
ATOM	5187	CB	PHE		46.203 19.911 26.314 1 00 54 32
ATOM	5188	CG	PHE	673	44.995 19.394 27.104 1 00 52 02
ATOM	5189		PHE	673 673	43.987 18.646 26 259 1 00 52.92
		-171	FUL	673	43 399 17 455
					26.728 1.00 53.49
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MOTA	5190	CD2	PHE	673	43.624	19.109	24.999	1.00 51.61
MOTA	5191	CE1	PHE	673	42.468	16.779	25.957	1.00 50.49
ATOM	5192	CE2		673	42.698	18.420	24.229	1.00 50.91
ATOM	5193	CZ	PHE	673	42.118	17.250	24.710	1.00 50.09
ATOM	5194	C	PHE	673	47.138	20.732	27.220	1.00 56.29
ATOM	5195	0	PHE	673	47.289	21.938	27.026	1.00 58.05
ATOM	5196	N	ASP	674	47.808	20.076	28.165	1.00 56.38
ATOM	5198	CA	ASP	674	48.703	20.772	29.104	1.00 56.12
MOTA	5199	CB	ASP	674	48.644	20.101	30.485	1.00 53.81
MOTA	5200	CG	ASP	674	47.299	20.234	31.152	1.00 52.48
ATOM	5201		ASP	674	46.715	19.188	31.504	1.00 50.25
ATOM	5202		ASP	674	46.844	21.384	31.337	1.00 51.16
MOTA	5203	С	ASP	674	50.182	20.886	28.706	1.00 57.07
ATOM	5204	0	ASP	674	51.010	21.273	29.541	1.00 56.00
MOTA	5205	N	ARG	675	50.525	20.526	27.468	1.00 57.28
MOTA	5207	CA	ARG	675	51.915	20.576	26.995	1.00 55.64
ATOM	5208	CB	ARG	675	52 341	22.020	26.692	1.00 58.95
MOTA	5209	CG	ARG	675	51.542	22.678	25.569	1.00 66.91
MOTA	5210	CD	ARG	675	52.082	24.066	25.202	1.00 72.90
MOTA	5211	NE	ARG	675	53.360	24.019	24.482	1.00 75.10
ATOM	5213	CZ	ARG	675	54.096	25.089	24.181	1.00 73.61
ATOM	5214	NH1	ARG	675	53.687	26.301	24.536	1.00 71.27
ATOM	5217	NH2	ARG	675	55.250	24.943	23.540	1.00 72.12
ATOM	5220	С	ARG	675	52.853	19.932	28.017	1.00 53.25
MOTA	5221	O	ARG	675	53.988	20.366	28.211	1.00 52.13
MOTA	5222	N	ILE	676 .	52.359	18.883	28.664	1.00 51.44
MOTA	5224	CA	ILE	676	53.108	18.153	29.683	1.00 49.81
MO'I'A	5225	CB	ILE	676	52.241	17.944	30.958	1.00 46.07
MOTA	5226	CG2	ILE	676	52.804	16.844	31.856	1.00 40.98
MOTA	5227	CG1	ILE	676	52.129	19.257	31.721	1.00 43.31
MOTA	5228	CD1	ILE	676	51.324	19.147	32.963	1.00 45.02.
MOTA	5229	C	ILE	676	53.572	16.800	29.144	1.00 51.20
MOTA	5230	0	ILE	676	52.770	15.892	28.951	1.00 52.37
ATOM	5231	N	TYR	677	54.865	16.675	28.890	1.00 52.81
ATOM	5233	CA	TYR	677	55.412	15.429	28.383	1.00 53.96
MOTA	5234	CB	TYR	677	56.296	15.700	27.167	1.00 57.26
ATOM	5235	CG	TYR	677	55.524	16.175	25.951	1.00 64.10
MOTA	5236	CD1	TYR	677	55.229	17.532	25.762	1.00 65.60
ATOM	5237	CEl	TYR	677	54.514	17.965	24.634	1.00 67.15
ATOM	5238	CD2		677	55.085	15.263	24.985	1.00 66.29
ATOM	5239		TYR	677	54.376	15.680	23.862	1.00 67.34
ATOM	5240	CZ	TYR	677	54.095	17.028	23.692	1.00 69.24
ATOM	5241	OH	TYR	6 <b>7</b> 7	53.399	17.414	22.573	1.00 73.55
ATOM	5243	C	TYR	677	56.192	14.713	29.482	1.00 52.30
ATOM	5244	0	TYR	677	57.053	15.309	30.124	1.00 53.73
MOTA	5245	N	THR	678	55.830	13.461	29.748	1.00 48.95
MOTA	5247	CA	THR	678	56.505	12.659	30.760	1.00 45.99
MOTA	5248	CB	THR	678	55.729	12.634	32.107	1.00 46.04
ATOM	5249		THR	678	54.663	11.676	32.046	1.00 49.79
ATOM	5251		THR	678	55.160	14.010	32.429	1.00 45.58
ATOM	5252	C	THR	678	56.656	11.221	30.261	1.00 43.81
ATOM	5253	0	THR	678	56.231	10.888	29.158	1.00 45.12

3	
ATOM 5254 N HIS 67	0
ATOM 5256 CA HTS CO	37.250 10.359 31 07
A1UM 5257 CB 1170	57.414 8.977 30 575 1.00 41.50
5258 CG 1170	9 58.390 8 353 30.687 1.00 38.39
ATOM 5259 CD2 UTS	59 700 51.603 1.00 38 62
ATOM -	60 456 31.524 1.00 41 51
ATOM 5262 CD 475	60 715 - 32.2/3 1.00 40 13
ATOM CEL HIS 670	61 880 30.613 1.00 47 70
ATOM 52C5 HIS 679	61 747 30.806 1.00 39 44
ATOM 5355 HIS 679	56 060 31.807 1.00 41 37
HIS 670	55 222 8.279 30.720 1 00 32 5-
ATOM 5367 N GLN 680	55.303 7.215 30.137 1 00 42 73
JAON CA GLN COO	8.863 31.429 1 00 32
52/0 CB GLN 600	53.773 8.290 31.483 1.00 33.84
AMON GG GLN 680	23.021 8 705 52
5272 CD GLN 600	53.518 8 005 - 2.00 38.21
5273 OE1 GIM	53.651 6.477 33 25 1.00 42.17
5274 NE2 GIN CO.	52.686 5.737 34 3-
A10M 5277 C 0734	54.860 6.070 33.55
ATOM 5278 0 CT	53.012 8 674 33.364 1.00 37.17
5279 N CER	52.220 7 993 0 1.00 39.33
ATOM 5281 CA (75)	53.299 9.854 20 75 1.00 40.26
ATOM 5282 CB CBD	52 636 10 251 22 1.00 38.00
ATOM 5283 OC 377	52 963 11 600 25.441 1.00 37.44
ATOM 5285 C GPR	54 340 28.078 1.00 37 67
ATOM 5286 0 577	53 096 28.102 1.00 34 03
ATOM 5287 W 581	52 302 27.356 1.00 38 20
ATOM 5289 33 105 682	54 363 26.510 1.00 39 41
ATOM 5300 101 082	54 920 ~ 27.431 1.00 36 91
ATOM 5303 101	56 404 - 20.495 1.30 36 43
ATOM - BB2	57 300 20.765 1.00 37 10
ATOM GRO	58 529 25.968 1.00 40 09
ATOM 5304 " 682	56 55 45.959 1 00 41 5
ATOM FOOT ASP 682	25.352 7 00 70
ATOM 530 ASP 682	54.180 6.561 26.645 7 00 35
5296 N VAL 603	53.71
3298 CA VAL 602	53.742 6.268 27.866 7.00 36.23
ATOM CB VAL 683	53.000 5.040 28.143 1.00 36.33
ATOM CG1 VAL 683	51 054 4.820 29.683 1.00 28
5301 CG2 VAI. 603	51.900 3.653 20 000 2.00 35.29
5302 C VAL 603	54.198 4.546 20 222
3303 O VAI. 603	5.067 37 305
3304 N TRD CO.	51.223 4.050 26 045
ALOM 5306 CA TRP 604	51.027 6.245 27 200 1.00 32.81
ATOM 5307 CR TPD 50	49.759 6.412 20 65 4.49
ATOM 5308 CG TRD	49.200 7 825 25 1.00 36.39
ATOM 5309 CD2 TDD	48.006 8.174 27 2.2 1.00 39.30
ATOM 5310 CE2 TTT	46.651 8.381 26.321 1.00 41.47
ATOM 5311 CF3 TDD	45.896 8 744 25 1.00 42.41
ATOM 5312 CD1 mpp	46.004 8 399 27 1.00 41.76
ATOM 5313 MB1 mm	48 010 27.627 1.00 42 06
ATOM 5315 COS	46 749 24.597 1.00 40 55
ATOM 684	44 522 - 24.1/5 1.00 42 22
ATOM - C43 TRP 684	44 639 25.315 1.00 41 35
	43 917 8.576 27.692 1.00 41 99
	43.917 8.933 26.541 1.00 41.07
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ATOM	5318	С	TRP	684	49.964	6.125	25.115	1.00 36.12
ATOM	5319	0	TRP	684	49.152	5.410	24.511	1.00 38.69
ATOM	5320	N	SER	685	51.029	6.690	24.534	1.00 33.48
ATOM	5322	CA	SER	685	51.395	6.491	23.130	1.00 26.49
ATOM	5323	CB	SER	685	52.636	7.300	22.802	1.00 23.40
MOTA	5324	OG	SER	685	52.403	8.688	22.992	1.00 30.31
MOTA	5326	С	SER	685	51.665	5.015	22.859	1.00 26.25
MOTA	5327	0	SER	685	51377	4.510	21.782	1.00 28.78
ATOM	5328	N	PHE	686	52.214	4.319	23.846	1.00 28.14
MOTA	5330	CA	PHE	686	52.470	2.884	23.727	1.00 28.53
ATOM	5331	CB	PHE	686	53.245	2.399	24.947	1.00 27.34
MOTA	5332	CG	PHE	686	53.567	0.937	24.917	1.00 29.91
MOTA	5333	CD1	PHE	686	54.424	0.419	23.942	1.00 29.23
ATOM	5334	CD2	PHE	686	53.016	0.075	25.861	1.00 28.28
MOTA	5335	CE1	PHE	686	54.725	-0.936	23.908	1.00 27.65
MOTA	5336	CE2	PHE	686	53.307	-1.274	25.840	1.00 27.18
MOTA	5337	CZ	PHE	686	54.166	-1.787	24.861	1.00 30.06
MOTA	5338	C	PHE	686	51.129	2.117	23.618	1.00 31.42
MOTA	5339	0	PHE	686	51.041	1.096	22.930	1.00 29.05
ATOM	5340	N	GLY	687	50.093	2.623	24.298	1.00 31.18
ATOM	5342	CA	GLY	687	48.783	2.000	24258	1.00 32.16
ATOM	5343	C	GLY	687	48.276	2.026	22.825	1.00 35.09
ATOM	5344	0	GLY	687	47.805	1.011	22.289	1.00 36.38
MOTA	5345	IJ	VAL	688	48.378	3.188	22.186	1.00 33.72
MOTA	5347	CA	VAL	688	47.949	3.307	20.808	1.00 30.28
MOTA	5348	CB	VAL	688	47.996	4.761	20.322	1.00 28.62
ATOM	5349	CG1	VAL	688	47.433	4.862	18.905	1.00 26.79
ATOM	5350		VAL	688	47.202	5.645	21.275	1.00 26.40
ATOM	5351	C	VAL	588	48.823	2.406	19.930	1.00 30.01
ATOM	5352	0	VAL	688	48.324	1.782	18.989	1.00 30.37
MOTA	5353	N	LEU	689	50.108	2.282	20.273	1.00 29.76
MOTA	5355	CA	LEU	689	51.022	1.418	19.510	1.00 29.37
ATOM	5356	CB	LEU	689	52.476	1.577	19.982	1.00 25.78
ATOM	5357	CG	LEU	689	53.564	0.944	19.097	1.00 23.00
ATOM	5358		LEU	689	54.855	1.741	19.153	1.00 24.44
ATOM	5359		LEU	689	53.823	-0.471	19.479	1.00 21.63
MOTA	5360	C	LEU	689	50.583	-0.043	19.634	1.00 29.98
MOTA	5361	0	LEU	689	50.708	-0.806	18.678	1.00 28.75
ATOM	5362	N	LEU	690	50.048	-0.409	20.803	1.00 32.38
ATOM	5364	CA	LEU	690	49.562	-1.764	21.060	1.00 32.66
ATOM	5365	CB	LEU	690	49.114	-1.929	22.517	1.00 32.33
ATOM	5366	CG	LEU	690	50.107	-2.192	23.658	1.00 32.00
ATOM	5367		LEU	690	49.330	-2.201	24.962	1.00 35.74
ATOM	5368	CD2		690	50.834	-3.513	23.475	1.00 30.76
ATOM	5369	C	LEU	690	48.369	-2.018	20.156	1.00 33.29
ATOM	5370	0	LEU	690	48.248	-3.079	19.550	1.00 35.08
ATOM	5371	N	TRP	691	47.490	-1.026	20.065	1.00 34.28
ATOM	5373	CA	TRP	691	46.304	-1.114	19.221	1.00 33.79
ATOM	5374	СВ	TRP	691	45.483	0.172	19.364	1.00 32.68
ATOM	5375	CG	TRP	691	44.147	0.144	18.669	1.00 31.23
ATOM	5376	CD2	TRP	691	43.888	0.490	17.312	1.00 28.11
MOTA	5377	CE2	TRP	691	42.506	0.310	17.089	1.00 29.96

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		5378	CE3	TRP 691	44 505
	rom	5379		TRP 691	14.000 0.949 16.257 1.00 28 70
		5380		TRP 691	19.208 1.00 29 27
	MO?	382	CZ2 '		18.265 1.00 30 99
	OM 5	383		TRP 691	41.909 0.555 15.845 1.00 00
	OM 5	384		RP 691	44.093 1.194 15.021 1.00 25
AT		385		RP 691	42.719 1.002 14 830 7 32
AT	OM 5	386			46./44 -1.319 17.763 1.00 2
ATO	OM 5	387			46.139 -2.088 17.029 1.00 57.12
ATO	OM 5	389			47.817 -0.636 17.366 1.00 33.88
ATO		390			48.355 _0 333
ATO		391	_	LU 692	49.532
ATO		392		LU 692	49 139
ATC		93		LU 692	50.318 2 505 1.00 32.63
ATO		94	OE1 GI		51 150 2 045
ATO		95	OE2 GI		50 430 3 227 10.301 1.00 37.81
ATO			C GI	_	48.810 -2 118 15 55
ATO			O GI		48 589 -2 570
ATO			N IL	E 693	49.439 -2.700 17.344 1.00 37.26
ATO			CA IL	E 693	49.944 -4.153
ATON			CB IL	E 693	50 843
ATOM			CG2 IL	E 693	51 275
			G1 IL		53 001 17.400 1.00 36.03
ATOM	_		D1 IL	E 693	52 234 17.669 1.00 34.66
ATOM		-	LLI		48 610 35.874 18.943 1.00 35.52
ATOM			ILE		18 700 15.153 16.232 1.00 34.29
ATOM			PHE		47 007 15.281 1.00 33.66
MOTA		8 C	A PHE		16 722 17.127 1.00 34.44
ATOM		9 C	в рне		17.082 1.00 35 42
ATOM	541	0 C	G PHE		18.490 1.00 35 36
ATOM	541	1 C	D1 PHE		19.428 1 00 3= 36
ATOM	541:	2 C1	D2 PHE	694	20.389 1 00 33 07
ATOM	541	3 C'1	E1 PHE	694	47.574 -8.111 19.237 1 00 31 74
ATOM	5414	CI	E2 PHE	694	48.837 -6.539 21.137 1.00 31 01
ATOM	5415	C2		694	48.614 -8.643 19.982 1 00 31 64
ATOM	5416		PHE	694	49.254 -7.855 20.934 1.00 31 84
MOTA	5417	0	PHE		45.688 -5.771 15.986 1 00 36 55
MOTA	5418		THR	694	44.844 -6.632 15.729 1 00 30 75
ATOM	5420			695	45.781 -4.626 15.313 1.00 75 -
ATOM	5421			695	44.898 -4.331 14 191 1 00 35.76
ATOM	5422			695	44.245 -2.929 14 299 1 00 34.86
ATOM	5424			695	45.246 -1.909 14 211 1 22
ATOM	5425	C C	2 THR	695	43 497 2 1.00 31.61
ATOM	5426		THR	695	45 766 4 436 15.003 1.00 29.90
ATOM	5427	0	THR	695	45 333 4 05 12.754 1.00 35.95
ATOM		N	LEU	696	46 993 4 000
ATOM	5429	CA	LEU	696	47 979 -5 100 34.68
ATOM	5430	CB	LEU	696	47 622 6 224
	5431	CG	LEU	696	47 493 7 657
ATOM ATOM	5432	CD1	LEU	696	47 315 0 77 11.030 1.00 30.89
	5433		LEU	696	48 718 7 22 10.785 1.00 31.30
ATOM	5434	C	LEU	696	48 280 2 222
ATOM	5435	0	LEU	696	48 259 3 222 11.197 1.00 32.43
ATOM	5436	N	GLY	697	49 507 9.965 1.00 31.48
				- *	48.597 -2.768 11.867 1.00 33.65

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-1.529 ATOM 5438 CA GLY 697 48.940 11.188 1.00 32.78 ATOM 5439 С GLY 697 47.742 -0.641 10.960 1.00 33.06 MOTA 5440 697 47.728 0.172 10.048 0 GLY 1.00 34.74 ATOM 5441 698 46.719 -0.798 11.782 1.00 35.53 N GLY CA 11.612 ATOM 5443 GLY 698 45.531 0.009 1.00 36.87 ATOM 5444 С GLY 698 45.771 1.496 11.753 1.00 34.92 **ATOM** 5445 0 GLY 698 46.779 1.926 12.299 1.00 34.08 ATOM 699 44.814 5446 SER 2.271 11.265 1.00 36.45 N ATOM 5448 CA SER 699 44.858 3.725 11.318 1.00 35.36 MOTA 5449 CB SER 699 44.363 4.290 9.995 1.00 34.58 MOTA 5450 699 OG SER 44.126 5.684 10.087 1.00 41.43 MOTA 5452 С SER 699 43.927 4.146 12.451 1.00 36.53 MOTA 5453 0 SER 699 42.734 3.812 12.438 1.00 37.58 ATOM 5454 PRO 700 4.799 N 44.471 13.491 1.00 36.03 ATOM 5455 CDPRO 700 45.896 5.028 13.776 1.00 34.58 ATOM 5456 CA PRO 700 43.630 5.228 14.611 1.00 35.47 ATOM 5457 CB PRO 700 44.655 5.573 15.694 1.00 34.59 **ATOM** 5458 CG PRO 700 45.840 5.990 14.919 1.00 34.18 **ATOM** 5459 С PRO 700 42.742 6.411 14.247 1.00 34.66 ATOM 5460 O PRO 700 43.194 7..363 13.616 1.00 34.39 ATOM 5461 N TYR 701 41.462 6 293 14.588 1.00 34.11 **ATOM** 5463 CA TYR 701 40.459 7.324 14.338 1.00 33.11 **ATOM** 5464 CB TYR 701 40.713 8..548 15.225 1.00 38.13 **ATOM** 5465 CG TYR 701 40.552 16.706 8.272 1.00 43.52 ATOM 5466 CD1 TYR 701 41.538 8.637 17.616 1.00 14.79 **ATOM** 546? CE1 TYR 701 41.387 8.391 18.978 1.00 49.99 MOTA 54*E*8 CD2 TYR 701 . 39.405 1.00 47.59 7.647 17.197 MOTA 5469 CE2 TYR 701 39.245 7.395 18.552 1.00 49 15 MOTA 5470 CZTYR 701 40.237 7.770 19.444 1.00 50.84 MOTA TYR 5471 701 40.091 OH 7.539 20.804 1.00 54.00 MOTA 701 5473 C TYR 40.389 7.736 12.877 1.00 30.95 8.900 ATOM 5474 TYR 701 40.597 12.534 O 1.00 30.64 40.096 **ATOM** 702 5475 N PRO 6.773 11.985 1.00 30.06 **ATOM** 5476 39.887 CD PRO 702 5.336 12.192 1.00 25.47 ATOM 5477 702 CA PRO 40.014 7.112 10.561 1.00 29.36 ATOM 5478 702 CB PRO 39.836 5.744 9.899 1.00 25.86 MOTA 5479 CG PRO 702 39.185 10.929 4.946 1.00 24.42 MOTA 5480 C PRO 702 38.859 8.045 10.256 1.00 31.49 MOTA 5481 0 PRO 702 37.716 7.794 10.654 1.00 33.50 MOTA N 5482 GLY 703 39.194 9.592 9.151 1.00 30.85 MOTA 5484 CA GLY 703 38.210 10.149 9.212 1.00 27.67 ATOM 703 5485 С GLY 37.9B5 11.230 10.250 1.00 27.39 ATOM 5486 GLY 703 9.981 0 37.270 12.194 1.00 26.56 ATOM 5487 N VAL 704 38.627 11.100 11.412 1.00 27.05 MOTA 5489 CA VAL 704 38.466 12.053 12.505 1.00 28.50 ATOM 5490 CB VAL 704 38.576 11.364 13.876 1.00 28.95 ATOM 5491 CG1 VAL 704 38.509 12.397 14.990 1.00 29.36 MOTA 5492 CG2 VAL 704 37.475 10.338 14.045 1.00 29.64 MOTA 5493 C VAL 704 39.473 13.194 12.493 1.00 30.95 MOTA 5494 0 VAL 704 40.669 12.977 12.661 1.00 32.90 MOTA 705 5495 N PRO 39.001 14.428 12.269 1.00 31.09 MOTA 5496 CD PRO 705 37.682 14.795 11.728 1.00 31.49



7 TOM	
ATOM 5497 CA PRO 705	39 026
ATOM 5498 CB PRO 705	15.561 12.255 1 00 29 66
ATOM 5499 CG PPO 705	10.618 11.477 1 00 30 16
ATOM 5500 C PRO 705	37.720 16.289 11 778 1 20 22
ATOM 5501 O PRO 305	40.334 16.028 13.654
ATOM 5502 N VAI 705	39.693 15.695 14.659 1.00
ATOM 5504 CD 100	41.396 16.828 13.690 1.00 24.77
ATOM SEAR OF	41 976 17 755
ATOM 5506 CC3 1155	43.023 19.450
706	43.680 18.003
ATOM 5500	44.058 17.040 1.00 37.79
ATOM FESS VAL 706	10 077
706 VAL 706	41.052 17.500 15.943 1.00 38.21
1\TOM 577	10 000 17.130 1.00 37.65
707 - CA GLU 707	30 045 15.734 15.467 1.00 40 27
ATOM	30 106 324 1.00 40.57
ATOM 5514 C GLU 707	15.499 1 00 10 55
ATOM 5515 O GLU 707	10.288 16.958 1.00 41 60
5516 N GLU 708	18.158 1.00 41 70
ATOM 5518 CA GLU 700	37.784 17.311 16.143 1.00 42 54
ATOM 5519 CB CTT	36.947 16.210 16 576 3 00
ATOM 5520 CG GLU 708	30 509 15.398 15 367 1 00
ATOM FED	35.687 16.219 14.381 7.00
ATOM 5522 OE1 GIH 700	34.511 16.891 15.042 7.00
ATOM 5523 OFF 708	33.856 16.249 15 899 1 66 55.51
ATOM 5524 C	34.244 18.067 14 214 1 22
ATOM 5525 0 553	37.661 15.338 17.500 7.00 60.06
ATOM 5526 N	37 050 14 300
ATOM 5528 Ch	38.960 15.12
ATOM 5529 CD	39.768 14 346 30 33
ATOM 5530	41,212 14, 242
709 LEU 709	42.037 13.350 12.55 1.00 34.99
Amore 709	41.619 11 010 1.00 31.80
ATOM 5532 - 709	43.495 12 722
ATOM FEET 709	39 751 15 000
ATOM 5709	39.646 14 215 13.363 L.00 39.26
710	39.872 16.337 20.714 1.00 37.71
CA PHE 710	36 969 10.327 19.691 1.00 38.62
ATOM 5538 CB PHE 710	40 016 -7.068 20.942 1.00 41.82
ATOM 5539 CG PHE 710	41 303 10.567 20.688 1.00 42.02
710 5540 CD1 PHE 710	10.938 20.206 1.00 43 91
710F1 5541 CD2 PHE 710	10.043 20.242 1 00 47 07
5542 CE1 PHE 710	42 774 20.234 19.718 1.00 42.91
ATOM 5543 CE2 PHE 710	10.401 19.793 1 00 40 22
ATOM 5544 CZ PHE 710	42.890 20.602 19.267 1.00 46 73
ATOM 5545 C PHE 710	43.942 19.681 19.307 1 30 48 40
ATOM 5546 O DHE 710	38.568 16.787 21 600 1 22
ATOM 5547 N LVS 711	38.593 16.502 22 904 1 00
ATOM 5549 CA LVC 731	37.452 16.790 20 969 1 20
ATOM 5550 CD	36.148 16.539 21 569 1 22
ATOM 5551 CG	35.029 16.855 20 577 1 00 42.60
ATOM SEED OF THE	33 661 16 72
ATOM 5552 OF	32 560 17 205
ATOM 5554 VG	31 212 16 20: 20.263 1.00 49.23
710M 5554 NZ LYS 711	30 078 17 000
	30.0/8 17.204 19.987 1.00 56.56

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MOTA	5558	C	LYS	711	36.045	15.105	22.084		41.50
MOTA	5559	0	LYS	711	35.589	14.875	23.202		41.06
MOTA	5560	N	LEU	712	36.489	14.144	21.282	1.00	41.61
ATOM	5562	CA	LEU	712	36.463	12.737	21.687	1.00	43.22
ATOM	5563	CB	LEU	712	37.070	11.841	20.600	1.00	41.69
ATOM	5564	CG	LEU	712	36.246	11.404	19.397	1.00	38.07
ATOM	5565	CD1	LEU	712	37.071	10.460	18.527	1.00	34.55
ATOM	5566	CD2	LEU	712	34.990	10.714	19.891	1.00	37.28
ATOM	5567	С	LEU	712	37.253	12.536	22.982	1.00	43.94
ATOM	5568	0	LEU	712	36.804	11.832	23.900	1.00	41.71
ATOM	5569	N	LEU	713	38.444	13.129	23.029	1.00	45.26
ATOM	5571	CA	LEU	713	39.318	13.022	24.191		46.47
ATOM	5572	CB	LEU	713	40.647	13 728	23.925		46.32
ATOM	5573	CG	LEU	713	41.524	13.012	22.889		44.05
ATOM	5574		LEU	713	42.853	13.737	22.734		39.96
ATOM	5575		LEU	713	41 758	11.571	23.328		41.78
ATOM	5576	C	LEU	713	38.665	13.519	25.477		47.50
ATOM	5577	Ö	LEU	713	38.630	12.789	26.472		48.26
ATOM	5578	N	LYS	714	38.098	14.725	25.440		47.08
ATOM	5580	CA	LYS	714	37.41.9		26.600		45.59
ATOM	5581	CB	LYS	714.	36.974	16.727.	26.293		47.53
ATOM	5582	CG	LYS	714	38.126	17.661	26.064		51.33
ATOM	5583	CD	LYS	714	37.647				
ATOM	5584	CE	LYS	714		19.044	25.689		59.12
ATOM	5585	NZ.			38.836	19.917	25.273		64.39
ATOM	5589	C C	LYS	714	39.843	20.072	26.370		66.31
ATOM	5590	0	LYS LYS	714	36.217	14.476	27.056		44.19
MOTA	5591	N	GLU	714	35.895	14.447	28.244		43.04
MOTA	5593	CA	GLU	715 715	35.565	13.805	26.112		43.89
ATOM	5594	CB	GLU	715	34.401	12.7976	26.424		44.12
ATOM	5595	CG	GLU	715	33.512	12.785	25.190		47.40
ATOM	5596	CD			32.860	14.053	24.623		52.31
ATOM			GLU	715	31.953	13.763	23.427		56.22
	5597		GLU	715	32.121	12.699	22.784		57.16
ATOM	5598	OE2	GLU	715	31.059	14.588	23.138		57.32
ATOM	5599	C.	GLU	715	34.809	11.605	26.956		42.47
MOTA	5600	0	GLU	715	33.964	10.718	27.094		41.03
ATOM	5601	N	GLY	716	36.101	11.419	27.201		41.06
ATOM	5603	CA	GLY	716	36.593	10.150	27.718		41.58
ATOM	5604	C	GLY	716	36.548	8.985	26.739		41.60
ATOM	5605	0	GLY	716	36.640	7.816	27.141		38.34
ATOM	5606	N	HIS	717	36.469	9.303	25.450		42.80
MOTA	5608	CA	HIS	717	36.398	8.278	24.420		45.03
ATOM	5609	CB	HIS	717	36.082	8.894	23.052		46.28
ATOM	5610	CG	HIS	717	35.987	7.887	21.940		48.73
MOTA	5611	CD2		717	34.941	7.157	21.483		48.67
ATOM	5612	ND1		717	37.071	7.521	21.169		49.33
ATOM	5614	CE1		717	36.701	6.607	20.290		45.65
ATOM	5615	NE2		717	35.410	6.370	20.460	1.00	45.87
MOTA	5617	С	HIS	717	37.662	7.448	24.324	1.00	46.84
ATOM	5618	0	HIS	717	38.767	7.980	24.319	1.00	48.06
MOTA	5619	N	ARG	718	37.478	6.138	24.217	1.00	48.75
ATOM	5621	CA	ARG	718	38.573	5.181	24.091	1.00	49.16

ATOM 5622 CB ARG 718 38.694 4.345 25.370 1.00 46.96 ATOM 5625 CD ARG 718 39.005 5.164 26.617 1.00 49.78 ATOM 5625 NE ARG 718 40.345 5.891 26.474 1.00 52.81 ATOM 5625 NE ARG 718 40.598 7.961 27.817 1.00 52.81 ATOM 5628 NH1 ARG 718 40.598 7.961 27.817 1.00 52.81 ATOM 5631 NH2 ARG 718 40.694 8.755 26.836 1.00 52.33 ATOM 5631 NH2 ARG 718 41.025 8.553 28.928 1.00 49.38 ATOM 5631 NH2 ARG 718 41.025 8.553 28.928 1.00 49.38 ATOM 5636 N MET 719 39.286 3.899 22.878 1.00 50.50 83 ATOM 5636 CB MET 719 39.286 3.899 22.136 1.00 50.58 ATOM 5636 CB MET 719 40.355 3.012 20.994 1.00 50.56 ATOM 5634 CB MET 719 40.355 3.012 20.994 1.00 48.85 ATOM 5636 CB MET 719 40.748 4.325 1.00 49.325 4.00 49.325 ATOM 5642 CB MET 719 42.152 4.119 18.335 1.00 43.25 ATOM 5642 CB MET 719 42.152 4.119 18.335 1.00 45.25 ATOM 5644 CB MET 719 38.649 1.671 21.312 1.00 51.07 ATOM 5644 CB MET 719 38.649 1.671 21.312 1.00 51.07 ATOM 5644 CB MET 719 38.649 1.671 21.312 1.00 51.07 ATOM 5645 CB ASP 720 37.797 1.096 20.462 1.00 53.92 ATOM 5645 CA ASP 720 37.797 1.096 20.462 1.00 53.92 ATOM 5645 CA ASP 720 37.797 1.096 20.462 1.00 53.92 ATOM 5645 CA ASP 720 37.254 0.253 20.548 1.00 59.95 ATOM 5655 CB ASP 720 37.254 0.253 20.548 1.00 59.95 ATOM 5655 CB ASP 720 37.254 0.253 20.548 1.00 59.95 ATOM 5655 CB ASP 720 37.254 0.253 20.548 1.00 55.90 ATOM 5655 CB ASP 720 37.254 0.253 20.548 1.00 55.89 ATOM 5655 CB ASP 720 37.254 0.253 20.548 1.00 55.89 ATOM 5655 CB ASP 720 37.254 0.253 20.548 1.00 55.89 ATOM 5656 CB ASP 720 37.254 0.253 20.548 1.00 55.89 ATOM 5657 CB ASP 720 34.951 1.316 20.312 1.00 56.66 ATOM 5657 CB ASP 720 34.951 1.316 20.312 1.00 56.66 ATOM 5657 CB ASP 720 34.951 1.316 20.312 1.00 56.66 ATOM 5657 CB ASP 720 34.951 1.316 20.312 1.00 56.95 ATOM 5659 CB ASP 720 34.951 1.316 20.312 1.00 56.66 ATOM 5659 CB ASP 720 34.951 1.316 20.312 1.00 56.66 ATOM 5650 CB ASP 720 34.951 1.316 20.312 1.00 56.66 ATOM 5650 CB ASP 720 38.366 ATOM 5650 CB ASP 720 38.366 ATOM 5650 CB ASP 720 38.366 ATOM 5650 CB ASP 721 38.364 ATOM 5650 CB ASP 722 39.957 CB ATOM 5650 CB ASP 72	2	77014			
ATOM 5623 CG ARC 718 30.005 5.164 26.617 1.00 46.96 ATOM 5625 NE ARG 718 40.344 5.891 26.474 1.00 52.81 ATOM 5627 CZ ARG 718 40.724 6.639 27.672 1.00 52.81 ATOM 5631 NH1 ARG 718 40.598 7.961 27.617 1.00 52.93 ATOM 5631 NH2 ARG 718 40.598 7.961 27.617 1.00 53.38 ATOM 5631 NH2 ARG 718 40.094 8.705 26.836 1.00 52.33 ATOM 5635 O ARG 718 38.257 4.293 22.878 1.00 53.38 ATOM 5635 O ARG 718 38.257 4.293 22.878 1.00 50.73 ATOM 5638 CA MET 719 39.286 3.899 22.136 1.00 50.73 ATOM 5638 CA MET 719 39.286 3.899 22.136 1.00 50.73 ATOM 5638 CA MET 719 40.355 3.012 20.094 1.00 48.85 ATOM 5640 CG MET 719 40.355 3.012 20.094 1.00 48.85 ATOM 5640 CG MET 719 40.365 3.012 20.094 1.00 48.85 ATOM 5641 SD MET 719 40.365 3.012 20.094 1.00 45.25 ATOM 5640 CG MET 719 39.086 3.072 20.948 1.00 50.83 ATOM 5640 CG MET 719 40.365 3.012 20.094 1.00 45.25 ATOM 5640 CG MET 719 40.365 3.012 20.094 1.00 45.25 ATOM 5640 CG MET 719 39.087 1.12 22.325 1.00 43.24 ATOM 5640 CG MET 719 39.087 1.12 22.325 1.00 48.22 ATOM 5640 CG MET 719 39.087 1.12 22.325 1.00 48.22 ATOM 5648 CB ASP 720 37.757 1.096 20.462 1.00 53.92 ATOM 5648 CB ASP 720 37.254 -0.253 20.648 1.00 53.92 ATOM 5650 ODI ASP 720 34.951 1.312 20.325 1.00 55.05 ATOM 5650 ODI ASP 720 34.951 1.312 20.325 1.00 55.05 ATOM 5650 ODI ASP 720 34.951 1.312 20.325 1.00 55.05 ATOM 5650 CC ASP 720 34.951 1.316 20.312 1.00 66.42 ATOM 5655 C Lys 721 38.006 2.450 21.304 1.00 55.28 ATOM 5656 C Lys 721 38.006 2.450 21.304 1.00 55.28 ATOM 5666 C Lys 721 38.006 2.450 21.304 1.00 56.42 ATOM 5666 C Lys 721 38.006 2.450 21.304 1.00 56.42 ATOM 5666 C Lys 721 38.006 2.450 21.304 1.00 56.42 ATOM 5666 C Lys 721 38.006 2.450 21.304 1.00 56.42 ATOM 5667 CB APRO 722 39.765 -6.48 8.501 1.00 56.72 ATOM 5668 C Lys 721 38.006 2.450 21.304 1.00 56.42 ATOM 5667 CB PRO 722 39.765 -6.48 8.501 1.00 56.72 ATOM 5668 C A Lys 721 38.006 2.450 21.304 1.00 56.40 3.204 ATOM 5668 C C Lys 721 38.006 2.450 21.304 1.00 56.40 3.204 ATOM 5668 C C Lys 721 38.006 2.450 21.304 1.00 56.10 57.204 ATOM 5668 C C Lys 721 38.006 2.450 21.304 1.00 56.70 5				ARG 7	18 20.00
ATOM 5624 CD ARC 718		302	3 CG	<b>&gt; -</b> -	4.345 25.370 1 00 46 05
ATOM 5625 NE ARG 718 40.7344 5.891 26.474 1.00 52.81 ATOM 5628 NH1 ARG 718 40.598 7.961 27.672 1.00 52.81 ATOM 5631 NH2 ARG 718 40.598 7.961 27.672 1.00 53.38 ATOM 5633 NH2 ARG 718 40.094 8.705 26.836 1.00 52.33 ATOM 5634 C ARG 718 38.257 4.293 22.878 1.00 50.73 ATOM 5635 O ARG 718 38.257 4.293 22.878 1.00 50.73 ATOM 5636 N MET 719 39.086 3.899 22.136 1.00 50.73 ATOM 5639 CB MET 719 39.086 3.072 20.948 1.00 50.63 ATOM 5639 CB MET 719 40.355 3.012 20.094 1.00 50.83 ATOM 5640 CG MET 719 40.748 4.325 19.438 1.00 48.85 ATOM 5641 SD MET 719 40.748 4.325 19.438 1.00 48.85 ATOM 5642 CE MET 719 43.471 4.066 19.465 1.00 43.24 ATOM 5643 C MET 719 38.089 1.671 21.312 1.00 51.07 ATOM 5644 C MET 719 38.089 1.671 21.312 1.00 51.07 ATOM 5646 C ASP 720 37.797 1.096 20.462 1.00 53.92 ATOM 5649 CG ASP 720 37.797 1.096 20.462 1.00 53.92 ATOM 5654 N ASP 720 37.797 1.096 20.462 1.00 53.92 ATOM 5654 C ASP 720 34.998 0.320 19.552 1.00 48.42 ATOM 5654 N LYS 721 38.4951 1.316 20.312 1.00 55.90 ATOM 5654 N LYS 721 38.4951 1.316 20.312 1.00 55.09 ATOM 5655 C LYS 721 38.409 1.190 20.027 1.00 56.49 ATOM 5656 C LYS 721 38.495 1.136 20.638 1.00 55.09 ATOM 5656 C LYS 721 38.449 -4.606 22.375 1.00 63.29 ATOM 5656 C LYS 721 38.449 -4.606 22.375 1.00 66.40 ATOM 5656 C LYS 721 38.449 -4.606 22.375 1.00 66.40 ATOM 5657 C B LYS 721 38.449 -4.606 22.375 1.00 66.40 ATOM 5656 C LYS 721 38.449 -4.606 22.375 1.00 66.40 ATOM 5657 C B LYS 721 38.449 -4.606 22.375 1.00 66.40 ATOM 5669 C B LYS 721 38.449 -4.606 22.375 1.00 66.40 ATOM 5669 C B LYS 721 38.449 -4.606 22.375 1.00 66.40 ATOM 5667 N PRO 722 40.133 -4.439 19.403 1.00 56.09 ATOM 5668 C B LYS 721 38.449 -6.873 22.141 1.00 65.72 ATOM 5669 C B LYS 721 38.449 -6.873 22.141 1.00 65.26 ATOM 5669 C B LYS 721 38.449 -6.873 22.141 1.00 65.09 ATOM 5669 C B LYS 721 38.449 -6.873 22.141 1.00 65.00 ATOM 5669 C B LYS 721 38.449 -6.873 22.141 1.00 65.00 ATOM 5669 C B LYS 721 38.449 -6.873 22.141 1.00 65.00 ATOM 5669 C B RO 722 40.445 3.768 18.509 1.00 55.16 ATOM 5668 C C A SR 723 39.456 -6.498 18.123 1.00 65.10 A		302	4 CD		5.164 26.617 1 00 40 ==
ATOM 5627 CZ ARG 718 40.598 7.961 27.817 1.00 53.99 ATOM 5631 NH2 ARG 718 40.598 7.961 27.817 1.00 53.33 ATOM 5631 NH2 ARG 718 40.598 8.705 26.836 1.00 52.33 ATOM 5634 C ARG 718 38.257 4.293 22.878 1.00 52.33 ATOM 5636 N MET 719 37.086 4.003 22.601 1.00 50.73 ATOM 5636 CR MET 719 39.286 3.889 22.601 1.00 50.73 ATOM 5639 CR MET 719 39.286 3.072 20.948 1.00 50.73 ATOM 5639 CR MET 719 40.355 3.013 20.094 1.00 50.86 ATOM 5640 CR MET 719 40.355 3.013 20.094 1.00 50.86 ATOM 5640 CR MET 719 40.748 4.325 19.438 1.00 54.25 ATOM 5641 C MET 719 40.748 4.325 19.438 1.00 45.25 ATOM 5642 CR MET 719 42.152 4.119 18.335 1.00 45.25 ATOM 5644 O MET 719 38.649 1.671 21.312 1.00 51.07 ATOM 5645 N ASP 720 37.797 1.096 20.622 1.00 51.07 ATOM 5646 CR ASP 720 37.797 1.096 20.662 1.00 51.07 ATOM 5647 CA ASP 720 37.797 1.096 20.662 1.00 53.92 ATOM 5648 CR ASP 720 37.274 -0.253 20.648 1.00 55.90 ATOM 5650 OD1 ASP 720 34.998 0.320 19.553 1.00 57.10 ATOM 5651 OD2 ASP 720 34.998 0.320 19.553 1.00 57.10 ATOM 5652 C ASP 720 34.998 0.320 19.553 1.00 57.08 ATOM 5653 O ASP 720 34.998 0.320 19.553 1.00 57.89 ATOM 5656 CA LYS 721 38.808 2.450 21.304 1.00 55.89 ATOM 5657 CR ASP 720 38.356 -1.343 20.638 1.00 55.89 ATOM 5658 CR LYS 721 38.808 2.450 21.304 1.00 56.40 ATOM 5657 CR LYS 721 38.808 2.450 21.304 1.00 56.09 ATOM 5658 CR LYS 721 38.808 2.450 21.304 1.00 56.09 ATOM 5659 CD LYS 721 38.808 -2.450 21.304 1.00 56.09 ATOM 5650 CR LYS 721 38.804 -4.532 19.403 1.00 56.00 ATOM 5660 CR LYS 721 38.804 -4.532 19.403 1.00 56.00 ATOM 5667 CR PRO 722 41.461 -3.968 19.835 1.00 57.16 ATOM 5668 CR PRO 722 41.401 -3.968 19.835 1.00 57.16 ATOM 5668 CR SER 723 39.079 -8.410 16.815 1.00 50.10 ATOM 5669 CA PRO 722 41.401 -3.968 19.835 1.00 59.26 ATOM 5669 CA PRO 722 41.401 -3.968 19.835 1.00 50.10 ATOM 5667 CB RO 722 40.28 -5.046 18.934 1.00 50.27 ATOM 5668 CB ASN 724 41.669 -1.245 15.543 1.00 68.26					8 5.891 26.474 1 00 53 00
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ATOM 5640 CB MET 719		2030		• 4.	39.286 3.800 27.601 1.00 51.78
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ATOM 5641 SD MET 719	ATC	· ·		ET 719	40 355 20.948 1.00 50 56
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ATOM 5667 N PRO 722 40.133 -4.439 19.423 1.00 56.00 ATOM 5668 CD PRO 722 41.461 -3.968 19.836 1.00 53.72 ATOM 5670 CB PRO 722 40.208 -5.046 18.094 1.00 51.82 ATOM 5671 CG PRO 722 42.143 -3.768 18.501 1.00 49.09 ATOM 5673 O PRO 722 42.143 -3.768 18.501 1.00 49.06 ATOM 5674 N SER 723 39.678 -7.120 19.188 1.00 48.82 ATOM 5676 CA SER 723 39.453 -7.020 16.945 1.00 49.87 ATOM 5677 CB SER 723 39.079 -8.410 16.814 1.00 50.27 ATOM 5680 C SER 723 39.273 -8.323 14.404 1.00 48.93 ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 51.33 ATOM 5682 N ASN 724 40.445 -10.284 17.551 1.00 54.65 ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76 ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 58.96 ATOM 5687 OD1 ASN 724 41.698 -12.345 15.543 1.00 62.08				721	38 930 24.156 1.00 75 61
ATOM 5668 CD PRO 722				721	37 994 1.241 19.985 1.00 56 00
ATOM 5669 CA PRO 722 41.461 -3.968 19.836 1.00 53.72  ATOM 5670 CB PRO 722 40.208 -5.046 18.094 1.00 51.82  ATOM 5671 CG PRO 722 42.143 -3.768 18.501 1.00 49.09  ATOM 5673 O PRO 722 39.765 -6.498 18.123 1.00 50.10  ATOM 5674 N SER 723 39.678 -7.120 19.188 1.00 48.82  ATOM 5676 CA SER 723 39.079 -8.410 16.814 1.00 50.27  ATOM 5678 OG SER 723 38.396 -8.643 15.473 1.00 49.87  ATOM 5678 OG SER 723 39.273 -8.323 14.404 1.00 48.93  ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 51.33  ATOM 5682 N ASN 724 40.445 -10.284 17.551 1.00 54.65  ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76  ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08		_	PRO	722	40 122 19.403 1.00 59 26
ATOM 5670 CB PRO 722		_	D PRO	722	19.423 1 00 54 30
ATOM 5670 CB PRO 722 41.702 -4.953 17.759 1.00 49.09 ATOM 5672 C PRO 722 42.143 -3.768 18.501 1.00 49.06 ATOM 5673 O PRO 722 39.765 -6.498 18.123 1.00 50.10 ATOM 5674 N SER 723 39.678 -7.120 19.188 1.00 48.82 ATOM 5676 CA SER 723 39.079 -8.410 16.814 1.00 50.27 ATOM 5678 OG SER 723 38.396 -8.643 15.473 1.00 48.56 ATOM 5680 C SER 723 39.273 -8.323 14.404 1.00 48.93 ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 48.93 ATOM 5682 N ASN 724 40.445 -10.284 17.551 1.00 51.18 ATOM 5685 CB ASN 724 40.445 -10.284 17.551 1.00 54.65 ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08		_	A PRO		19.836 1 00 53 55
ATOM 5671 CG PRO 722 42.143 -3.768 18.501 1.00 49.09 ATOM 5673 O PRO 722 39.765 -6.498 18.123 1.00 50.10 ATOM 5674 N SER 723 39.678 -7.120 19.188 1.00 48.82 ATOM 5676 CA SER 723 39.079 -8.410 16.814 1.00 49.87 ATOM 5677 CB SER 723 38.396 -8.643 15.473 1.00 48.56 ATOM 5680 C SER 723 39.273 -8.323 14.404 1.00 48.93 ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 51.33 ATOM 5682 N ASN 724 40.445 -10.284 17.551 1.00 54.65 ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76 ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08		_	_		10.208 -5.046 18.094 1 00 51 72
ATOM 5672 C PRO 722 39.765 -6.498 18.501 1.00 49.06 ATOM 5673 O PRO 722 39.678 -7.120 19.188 1.00 50.10 ATOM 5674 N SER 723 39.678 -7.120 19.188 1.00 48.82 ATOM 5676 CA SER 723 39.079 -8.410 16.814 1.00 50.27 ATOM 5678 OG SER 723 38.396 -8.643 15.473 1.00 48.56 ATOM 5680 C SER 723 39.273 -8.323 14.404 1.00 48.93 ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 51.33 ATOM 5682 N ASN 724 40.445 -10.284 17.551 1.00 51.18 ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76 ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08			G PRO		12.702 -4.953 17.759 1 00 40 00
ATOM 5673 O PRO 722 39.765 -6.498 18.123 1.00 50.10  ATOM 5674 N SER 723 39.678 -7.120 19.188 1.00 48.82  ATOM 5676 CA SER 723 39.453 -7.020 16.945 1.00 49.87  ATOM 5677 CB SER 723 39.079 -8.410 16.814 1.00 50.27  ATOM 5678 OG SER 723 38.396 -8.643 15.473 1.00 48.56  ATOM 5680 C SER 723 39.273 -8.323 14.404 1.00 48.93  ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 51.33  ATOM 5682 N ASN 724 40.445 -10.284 17.551 1.00 51.18  ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76  ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08					42.143 -3.768 18 501 1 00
ATOM 5676 CA SER 723 39.453 -7.020 16.945 1.00 48.82 ATOM 5677 CB SER 723 39.079 -8.410 16.814 1.00 50.27 ATOM 5678 OG SER 723 38.396 -8.643 15.473 1.00 48.56 ATOM 5680 C SER 723 39.273 -8.323 14.404 1.00 48.93 ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 51.33 ATOM 5682 N ASN 724 41.400 -8.679 16.311 1.00 51.18 ATOM 5685 CB ASN 724 40.445 -10.284 17.551 1.00 54.65 ATOM 5686 CG ASN 724 41.673 -11.062 17.706 1.00 56.76 ATOM 5687 OD1 ASN 724 41.698 -12.345 15.543 1.00 62.08			PRO		39.765 -6.498 18.123 1 00 50 10
ATOM 5676 CA SER 723 39.079 -8.410 16.814 1.00 49.87  ATOM 5677 CB SER 723 38.396 -8.643 15.473 1.00 48.56  ATOM 5680 C SER 723 39.273 -8.323 14.404 1.00 48.93  ATOM 5681 O SER 723 40.414 -9.144 16.872 1.00 51.33  ATOM 5682 N ASN 724 41.400 -8.679 16.311 1.00 51.18  ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76  ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08					33.678 -7.120 19.188 1 00 40 20
ATOM 5677 CB SER 723 39.079 -8.410 16.814 1.00 50.27  ATOM 5678 OG SER 723 39.273 -8.323 14.404 1.00 48.56  ATOM 5680 C SER 723 40.414 -9.144 16.872 1.00 51.33  ATOM 5681 O SER 723 41.400 -8.679 16.311 1.00 51.18  ATOM 5682 N ASN 724 40.445 -10.284 17.551 1.00 54.65  ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76  ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08		5676 CZ			33.433 -7.020 16 045
ATOM 5678 OG SER 723 38.396 -8.643 15.473 1.00 48.56 ATOM 5680 C SER 723 40.414 -9.144 16.872 1.00 51.33 ATOM 5681 O SER 723 41.400 -8.679 16.311 1.00 51.18 ATOM 5684 CA ASN 724 40.445 -10.284 17.551 1.00 54.65 ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76 ATOM 5686 CG ASN 724 41.698 -12.345 15.543 1.00 62.08					39.079 -8.410 16.814
ATOM 5680 C SER 723	ATOM				38.396 -8.643 15 473
ATOM 5681 O SER 723					39.273 -8.323 14 404
ATOM 5682 N ASN 724 41.400 -8.679 16.311 1.00 51.13  ATOM 5684 CA ASN 724 40.445 -10.284 17.551 1.00 54.65  ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76  ATOM 5686 CG ASN 724 42.370 -11.286 16.359 1.00 58.96  ATOM 5687 OD1 ASN 724 41.645 -12.345 15.543 1.00 62.08	ATOM	F F S -			40.414 -9.144 16.072
ATOM 5684 CA ASN 724 40.445 -10.284 17.551 1.00 51.18 ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 56.76 ATOM 5686 CG ASN 724 42.370 -11.286 16.359 1.00 58.96 ATOM 5687 OD1 ASN 724 41.645 -12.345 15.543 1.00 62.08					41,400 0 572 1.00 51.33
ATOM 5685 CB ASN 724 41.673 -11.062 17.706 1.00 54.65 ATOM 5686 CG ASN 724 42.370 -11.286 16.359 1.00 58.96 ATOM 5687 OD1 ASN 724 41.645 -12.345 15.543 1.00 62.08		550.			40.445 -10 204 10.311 1.00 51.18
ATOM 5686 CG ASN 724 42.370 -11.286 16.359 1.00 58.96 ATOM 5687 OD1 ASN 724 41.698 -12.345 15.543 1.00 62.08	3 550				41.673 -11.000 17.551 1.00 54.65
ATOM 5687 OD1 ASN 724 41.698 -12.345 15.359 1.00 58.96 41.645 -13.500 15.543 1.00 62.08	T. CO.			724	42.370 -11 206 1.00 56.76
ODI ASN 724 41.645 -13.543 1.00 62.08	7.000		ASN		41.698 -12 245 16.359 1.00 58.96
15.948 1.00 67.56		2381 OD	ASN	724	41.645 -12.500 15.543 1.00 62.08
					15.948 1.00 67.56

WO 98/07835

ATOM	5688	ND2	ASN	724	41.154	-11.960	14.403	1.00 60.12
MOTA	5691	C	ASN	724	42.622	-10.381	18.683	1.00 57.26
ATOM	5692	0	ASN	724	43.786	-10.131	18.383	1.00 58.40
MOTA	5693	N	CYS	725	42.089	-10.045	19.845	1.00 57.58
MOTA	5695	CA	CYS	725	42.852	-9.418	20.908	1.00 57.02
MOTA	5696	CB	CYS	725	42.835	-7.885	20.803	1.00 55.65
MOTA	5697	SG	CYS	725	43.782	-7.034	22.119	1.00 52.17
MOTA	5698	C	CYS	725	42.158	-9.884	22.177	1.00 56.53
MOTA	5699	0	CYS	725	40.927	-9.954	22.240	1.00 55.99
MOTA	5700	N	THR	726	42.957	-10.279	23.155	1.00 56.09
ATOM	5702	CA	THR	726	42.453	-10.773	24.423	1.00 57.09
ATOM	5703	CB	THR	726	43.551	-11.579	25.129	1.00 57.12
ATOM	5704	OG1	THR	726	44 588	-10.696	25.562	1.00 59.14
ATOM	5706	CG2	THR	726	44.152	-12.587	24.154	1.00 55.09
ATOM	5707	C	THR	726	41.994	-9.608	25.288	1.00 57.58
ATOM	5708	0	THR	726	42.555	-8.518	25.195	1.00 58.49
ATOM	5709	N	ASN	727	40.979	-9.832	26.120	1.00 58.48
MOTA	5711	CA	ASN	727	40.482	-8.774	26.986	1.00 58.74
ATOM	5712	CB	ASN	727	39.331	-9.267	27.864	1.00 66.81
ATOM	5713	CG	ASN	727	39.674	-10.534	28.631	1.00 76.72
ATOM	5714	OD1	ASN	727	40.778	-10.689	29.161	1.00 80.48
ATOM	5715	ND2	ASN	727	38.716	-11.458	28.689	1.00 82.39
ATOM	5718	C	ASN	727	41.606	8.238	27.852	1.00 55.48
ATOM	5719	0	ASN	727	41.589	-7.080	28.255	1.00 51.24
MOTA	5720	N	GLU	728	42.589	-9.099	28.114	1.00 55.37
MOTA	5722	CA	GLU	728	43.757	-8.739	28.913	1.00 55.53
MOTA	5723	CB	GLU	728	44.611	-9.983	29.198	1.00 55.75
ATOM	5724	CG	GLU	728	45.881	-9.699	30.006	1.00 58.24
ATOM	5725	CD	GLU	728	46.606	-10.958	30.463	1.00 58.16
ATOM	5726	OE1	GLU	728	46.977	-11.796	29.611	1.00 56.39
ATOM	5727	OE2	GLU	728	46.816	-11.102	31.686	1.00 58.35
MOTA	5728	C	GLU	728	44.564	-7.685	28.153	1.00 54.11
ATOM	5729	9	GLU	728	44.790	-6.575	28.654	1.00 55.67
ATOM	5730	N	LEU	729	44.954	-8.020	26.926	1.00 49.65
MOTA	5732	CA	LEU	729	45.715	-7.106	26.086	1.00 46.10
ATOM	5733	CB	LEU	729	46.038	-7.766	24.742	1.00 39.77
ATOM	5734	CG	LEU	729	47.136	-8.836	24.848	1.00 36.12
ATOM	5735	CD1	LEU	729	47.118	-9.757	23.673	1.00 34.89
ATOM	5736		LEU	729	48.498	-8.193	24.987	1.00 33.47
ATOM	5737	C	LEU	729	44.950	-5.794	25.908	1.00 45.05
ATOM	5738	0	LEU	729	45.522	-4.713	26.019	1.00 45.58
ATOM	5739	N	TYR	730	43.640	-5.884	25.722	1.00 43.53
ATOM	5741	CA	TYR	730	42.831	-4.692	25.557	1.00 43.57
MOTA	5742	CB	TYR	730	41.414	-5.064	25.097	1.00 41.49
ATOM	5743	CG	TYR	730	40.492	-3.870	24.951	1.00 40.28
ATOM	5744	CD1		730	40.763	-2.865	24.013	1.00 36.86
ATOM	5745	CE1		730	39.937	-1.752	23.891	1.00 36.21
ATOM	5746			730	39.361	-3.730	25.768	1.00 39.44
ATOM	5747	CE2	TYR	730	38.522	-2.616	25.654	1.00 38.13
MOTA	5748	CZ	TYR	730	38.817	-1.632	24.712	1.00 38.79
ATOM	5749	OH	TYR	730	37.974	-0.542	24.575	1.00 40.32
ATOM	5751	C	TYR	730	42.806	-3.866	26.856	1.00 44.45

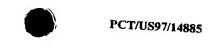
Д	MOTA	<b>-</b> 3	_			
	TOM	5752	_	TYR	730	42.786 -2.632 26 813
		5753		MET	731	-2.632 26.818 1 00 43 45
	TOM	5755	CA	MET	731	' * 334 /X NNC
A'	TOM	5756	CB	MET	731	42.805 -3.812 29 270
	TOM	5757	CG	MET		42.516 -4.748 30.447 1.00 48.59
A7	TOM	5758	SD		731	41.132 - 307 1.00 54.69
		5759	CE	MET	731	39.781 -4 100 50.398 1.00 62.68
		5760		MET	731	39.492 -4 013 -1.00 70.49
			С	MET	731	44 767 4.012 32.209 1.00 72 27
		5761	0	MET	731	44 320 29.450 1.00 46 48
		5762	N	MET	732	2.005 30.086 1 00 44 03
AT		764	CA	MET	732	45.202 -3.751 28.881 1 00 43 00
AT	_	765	CB i	MET	732	*0.538 -3.167 28 930
ATO		766		MET		*7.593 -4.104 28 322
ATO		767			732	49.028 3 500
ATO	~	768	`	ÆT	732	50.312
ATC		769		ET	732	50.547 -5 573 27.9/9 1.00 36.47
ATO	_			ET	732	46 474 373 29.530 1.00 41 29
ATO	_	770	O M	ET	732	46 005 28.188 1.00 42 08
	_	771	N M	ET	733	28.659 1 20 42 1
ATO	_	773	CA M	ET	73.3	27.054 1 00 43 14
ATO		774	CB M	ET	733	25.608 -0.609 26.257 1 00 42 24
ATO		7.5	CG M	ET	733	14.854 -0.877 24 847
ATO!	M 57	76	SD MI		733	45.607 -1.730 23 920
ATON			CE ME			44.669 -2.025 22 410
ATON	4 57		_		733	45.183
ATOM			_		733	44.820 0 200 = 1.00 28.12
ATOM					733	45.215 1 550
ATOM			∛ AR	•	734	44 712 27.196 1.00 43.78
ATOM			A AR	G 7	<b>'34</b>	42 002 27.555 1.00 42 59
ATOM		-	B AR	G 7	34	11 542 28.467 1.00 42 92
		_	G AR		34	28.966 1 (0.42.25
ATOM	_		D AR		34	20.753 -0.374 27.852 1.00 30 76
ATOM			E ARC		34	20.360 (1.763 26.959 1 20 47 02
ATOM	578	8 C			34	39.535 1.745 27 652 -
ATOM	578		H1 ARC			38.207 1.693 27 700
ATOM	579		H2 ARC		34	37.542 0.708 27 317 1 3
ATOM	579		ARG		34	37.534 2.642
ATOM	5796	_				43.719 1 305 1.00 53.24
ATOM	5797	_	ARG			43.610 2 578 25.030 1.00 42.42
ATOM	5799		ASP	. –		44.591 0 544
ATOM				73	5	45 464 30.187 1.00 41.40
ATOM	5800			73	5	46 333 31.286 1.00 43 33
	5801			73	5	0.194 31 755 1 00 15
ATOM	5802		1 ASP	73.	5	45 32.496 1.00 54 95
ATOM	5803	OD:	2 ASP	73		74.451 77 770
ATOM	5804	С	ASP	739		33.012 -0.900 33 345
ATOM	5805	0	ASP			40.365 2.107 30 840
ATOM	5806	N	CYS	735		46.484 3.124 31 543 1 7
ATOM	5808	CA	CYS	736		47.021 1.926 29 693 1 20
ATOM	5809	CB		736		47.896
ATOM	5810		CYS	736		48.545 3.460 1.00 35.90
ATOM		SG	CYS	736		49.634 1.007 27.858 1.00 33.62
ATOM	5811	C	CYS	736		47 100 28.104 1.00 33 92
	5812	0	CYS	736		47 653
ATOM	5813	N	TRP	737		45 703 28.830 1.00 35.59
ATOM	5815	CA	TRP	737		45.793 4.039 28.668 1 00 38 00
						44.906 5.156 28.372 1.00 40.14
SSSD/FF						

ATOM	5816	CB	TRP	737	43.910	4.766	27.274	1.00 40.93
MOTA	5817	CG	TRP	<b>7</b> 37	44.563	4.379	25.977	1.00 42.36
ATOM	5818	CD2		737	44.018	3.518	24.969	1.00 43.84
ATOM	5819	CE2		737	44.972	3.437	23.929	1.00 46.42
MOTA	5820	CE3		737	42.817	2.806	24.845	1.00 42.43
MOTA	5821	CD1		737	45.793	4.775	25.519	1.00 42.57
ATOM	5822	NE1		737	46.043	4.214	24.292	1.00 44.22
ATOM	5824	CZ2		737	44.756	2.666	22.773	1.00 44.97
MOTA	5825	CZ3		737	42.606	2.042	23.699	1.00 40.74
ATOM	5826	CH2		737	43.571	1.978	22.682	1.00 40.75
MOTA	5827	C	TRP	737	44.157	5.70€	29.584	1.00 40.62
ATOM	5828	0	TRP	737	43.085	6.285	29.437	1.00 41.37
ATOM	5829	N	HIS	738	44.706	5.533	30.783	1.00 42.09
ATOM	5831	C'A	HIS	738	44.044	6.059	31.966	1.00 43.78
ATOM	5832	CB	HIS	738	44.635	5.463	33.248	1.00 46.52
MOTA	5833	CG	HIS	738	43.878	5.844	34.486	1.00 52.24
MOTA	5834		HIS	738	43.599	7.053	35.025	1.00 50.95
MOTA	5835		HIS	738	43.271	4.914	35.299	1.00 56.16
ATOM	5837	CEI	HIS	738	42.643	5.536	36.285	1.00 57.23
MOTA	5838		HIS	738	42.827	6.835	36.141	1.00 53.22
MOTA	5840	C	HIS	738	44.183	7.577	31.964	1.00 42.81
ATOM	5841	0	HIS	738	45.235	8.093	31.654	1.00 42.12
MOTA	5842	M	ALA	739.	43.121	8.285	32.324	1.00 45.66
ATOM	5844	CA	ALA	739	43.130	9.750	32.350	1.00 49.42
ATOM	5845	CB	ALA	739	41.739	10.262	32.681	1.00 53.04
ATOM	5846	C	ALA	739	44.167	10.380	33.291	1.00 50.18
ATOM	5847	O	ALA	739 .	44.710	11.450	33.006	1.00 51.86
ATOM	5848	N	VAL	740	44.322	9.780	34.466	1.00 49.96
ATOM	5850	CA	VAL	740	45.299	10.219	35.467	1.00 50.17
ATOM	5851	CB	VAL	740	44.828	9.849	36.881	1.00 50.33
ATOM	5852		VAL	740	45.880	10.209	37.896	1.00 51.40
ATOM	5853		VAL	740	43.534	10.559	37.193	1.00 50.86
ATOM	5854	C	VAL	740	46.626	9.497	35.196	1.00 49.81
ATOM	5855	0	VAL	740	46.749	8.295	35.472	1.00 49.85
ATOM	5856	N	PRO	741	47.646	10.230	34.713	1.00 47.92
ATOM	5857	CD	PRO	741	47.618	11.683	34.476	1.00 46.97
ATOM	5858	CA	PRO	741	48.968	9.686	34.393	1.00 46.47
ATOM	5859	CB	PRO	741	49.796	10.941	34.134	1.00 44.38
ATOM	5860	CG	PRO	741	48.800	11.877	33.561	1.00 44.86
ATOM	5861	C	PRO	741	49.593	8.815	35.480	1.00 47.21
ATOM	5862	0	PRO	741	50.243	7.816	35.176	1.00 46.77
ATOM	5863	N	SER	742	49.380	9.181	36.741	1.00 48.87
ATOM	5865	CA	SER	742	49.939	8.430	37.860	1.00 50.19
ATOM	5866	CB	SER	742	49.753	9.203	39.166	1.00 51.87
ATOM	5867	OG	SER	742	48.389	9.514	39.391	1.00 54.19
ATOM	5869	C	SER	742	49.331	7.040	38.010	1.00 51.30
ATOM	5870	0	SER	742	49.863	6.192	38.723	1.00 51.14
ATOM	5871	N	GLN	743	48.207	6.814	37.343	1.00 53.07
ATOM	5873	CA	GLN	743	47.531	5.531	37.414	1.00 53.50
ATOM	5874	CB	GLN	743	46.015	5.745	37.548	1.00 59.34
ATOM	5875	CG	GLN	743	45.412	5.307	38.898	1.00 66.19
ATOM	5876	CD	GLN	743	46.133	5.896	40.106	1.00 70.07

7	MOTA	5877	OE1	GIN =	· 
A	TOM	5878		~~	46.750 5.170 40.885 1.00 73 R6
A	TOM	5881	_		46.047 7.300 1.00 73.86
	ma	5882	_	GLN 74	3 47.850 4 613 - 40.273 1.00 72.01
A	ma	5883		GLN 74	3 47.504 3 435 30.236 1.00 51.14
	T			ARG 74	4 48 484 3.425 36.266 1.00 51 79
		5885		ARG 74	4 48 848 3.153 35.196 1.00 48 31
		5886	CB ]	ARG 74.	4 49 326 - 343 34.027 1.00 45.49
		887	CG į	ARG 74.	32.869 1.00 40 33
		888	CD I	ARG 744	32.324 1 00 36 30
		889	NE A	LRG 744	31.262 1 00 20 55
	-	891		RG 744	8.203 30.961 1 00 39 05
AT		892	NH1 A	RG 744	9.409 30.547 1.00 30.50
AT		895	NH2 A	RG 744	9.700 30.357 1 00 36 05
ATO		898		RG 744	47.516 10.354 30 306
ATO		899		RG 744	30.016 3.454 34 452
ATC	DM 59	900			50.794 3.824 35 334 7 35
ATC		901			50.133 2.251 33 960
ATC		02	CA PR		49.248 1.559 32 022
ATO		03	CB PR		51.261 1:402 34 271
ATO		04			50.972 0.070
ATO	M 59				50.155 0.403 25 1.00 41.77
ATO	M 59				52.590 2.001 32.354 1.00 42.26
ATO					52.621 2.005 25 1.00 40.30
ATON					53.679 1 570 - 39.73
ATON		`			54 007 1 34.433 1.00 39 14
ATOM			CB THE		55.992 2 704 2 1.00 38.35
ATOM		•	GI THE		56 202 2.104 35.249 1.00 36.75
ATOM			G2 THR		55.477 3.000 35.769 1.00 32.25
ATOM	J J 1	_			55 560 36.341 1.00 30.31
ATOM				746	55 105 32.987 1.00 37.90
ATOM		_		747	56 400 32.938 1.00 37 99
ATOM		_		747	57 106 32.157 1.00 35.94
ATOM	5919			747	58 124 31.161 1.00 35.00
ATOM	5920			747	57 512 30.309 1.00 30.45
ATOM	592]		O1 PHE	747	56 050 27.14 29.142 1.00 27.61
ATOM	5922		2 PHE	747	57 460 28.103 1.00 23 68
ATOM	5923		1 PHE	747	56 353 29.094 1.00 27 97
ATOM	5924		2 PHE	747	56 960 27.033 1.00 23.56
ATOM	5925	CZ	PHE	747	28.027 1 00 25 02
ATOM	5926	С	PHE	747	26.995 1 00 ac ac
	5927	O	PHE	747	57 000 31.826 1.00 36 37
ATOM	5928	N	LYS	748	1.325 31.219 1 00 37 -
MOTA	5930	CA	LYS	748	38.1// -0.312 33.075 1 00 30 60
ATOM	5931	CB	LYS	748	38.797 -1.411 33.807 1 00 42 22
ATOM	5932	CG	LYS	748	39.433 -0.895 35.095 1 00 46 1-
ATOM	5933	CD	LYS		39.978 -1.991 35.984 1 00 54 5-
ATOM	5934	CE	LYS	748	60.794 -1.428 37 135 4 3-
ATOM	5935	NZ	LYS	748	61.239 -2.537 38 075 1 38
MOTA	5939	C	LYS	748	62.167 -2.025 39 120 1 22
MOTA	5940	0		748	57.723 -2.463 34 111 1 2
MOTA	5941	N	LYS	748	57.998 -3 664 - 2.00 42.78
ATOM	5943	CA	GLN	749	56,503 -1 000 37.97
ATOM	5944		GLN	749	55.365 -2.066 34.392 1.00 43.27
	13	CB	GLN	749	54.146 -2.056
					34.146 -2.056 35.146 1.00 47.37
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WO 98/07835

ATOM	5945	CG	GLN	749	54.236	-1.504	36.569	1.00 51.86
MOTA	5946	CD	GLN	749	53.036	-0.639	36.938	1.00 54.76
ATOM	5947	OE1	GLN	749	53.181	0.504	37.350	1.00 58.36
ATOM	5948	NE2	GLN	749	51.846	-1.179	36.769	1.00 59.25
MOTA	5951	C	GLN	749	55.006	-3.607	33.389	1.00 41.66
MOTA	5952	0	GLN	749	54.978	-4.841	33.355	1.00 40.25
MOTA	5953	N	LEU	750	54.759	-2.843	32.327	1.00 41.47
ATOM	5955	CA	LEU	750	54.398	-3.387	31.018	1.00 40.00
ATOM	5956	CB	LEU	750	54.366	-2.279	29.966	1.00 40.55
MOTA	5957	CG	LEU	750	53. <b>31</b> 6	-1.174	30.112	1.00 39.94
ATOM	5958	CD1	LEU	750	53.714		29.257	1.00 41.03
MOTA	5959	CD2	LEU	750	51.952	-1.696	29.722	1.00 37.80
ATOM	5960	С	LEU	750	55.383	-4.452	30.581	1.00 39.61
MOTA	5961	0	LEU	750	54.990	-5.470	30.027	1.00 42.08
ATOM	5962	N	VAL	751	56.670	-4.207	30.804	1.00 40.63
ATOM	5964	CA	VAL	751	57.691	-5.177	30.422	1.00 39.65
ATOM	5965	СВ	VAL	751	59.115	-4.639	30.677	1.00 33.44
ATOM	5966	CG1	VAL	751	60.142	-5.694	30.351	1.00 31.57
ATOM	5967	CG2	VAL	751	59.372	-3.433	29.825	1.00 25.19
ATOM	5968	C	VAL	751	57.458	-6.468	31.204	1.00 43.58
ATOM	5969	0	VAL	751	57.530	-7.563	30.646	1.00 44.81
ATOM	5970	N	GLU	752	57.116	- 6.339	32.481	1.00 46.24
ATOM	5972	CA	GLU	752	56.869	-7.518	33.301	1.00 50.55
MOTA	5973	СВ	GLU	752	56.781	-7.137	34.783	1.00 53.70
ATOM	5974	CG	GLU	752	58.090	-6.541	35.310	1.00 56.60
ATOM	5975	CD	GLU	752	58.079	-6.243	36.792	1.00 56.20
ATOM	5976	OE1	GLU	752	58.387	-5.092	37.178	1.00 53.45
ATOM	<b>597</b> 7	OE2	GLU	752	57.789	-7.170	37.573	1.00 60.28
MOTA	5978	С	GLU	752	55.622	-8.275	32.837	1.00 50.90
MOTA	5979	0	GLU	752	55.689	-9.474	32. <b>5</b> 55	1.00 51.03
ATOM	5980	N	ASP	753	54.501	-7.570	32.708	1.00 51.12
ATOM	5982	CA	ASP	753	53.251	-8.184	32.265	1.00 48.76
ATOM	5983	CB	ASP	753	52.122	-7.160	32.249	1.00 51.11
ATOM	5984	CG	ASP	753	51.646	-6.805	33.636	1.00 54.97
MOTA	5985	OD1	ASP	753	51.592	-7.715	34.495	1.00 58.37
ATOM	5986	OD2	ASP	753	51.319	-5.618	33.864	1.00 56.38
ATOM	5987	С	ASP	753	53.381	-8.790	30.881	1.00 48.02
MOTA	5988	0	ASP	753	52.991	-9.935	30.672	1.00 48.32
MOTA	5989	N	LEU	754	53.925	-8.020	29.940	1.00 45.16
MOTA	5991	CA	LEU	754	54.111	-8.490	28.571	1.00 44.82
MOTA	5992	CB	LEU	754	54.696	-7.387	27.691	1.00 42.70
ATOM	5993	CG	LEU	754	53.736	-6.263	27.298	1.00 42.92
ATOM	5994	CD1	LEU	754	54.500	-5.236	26.495	1.00 41.44
ATOM	5995	CD2	LEU	754	52.537	-6.822	26.502	1.00 42.86
MOTA	5996	С	LEU	754	55.001	-9.716	28.529	1.00 46.00
ATOM	5997	0	LEU	754		-10.606	27.708	1.00 45.88
ATOM	5998	N	ASP	755	55.975	-9.752	29.424	1.00 47.37
ATOM	6000	CA	ASP	755		-10.873	29.516	1.00 48.88
MOTA	6001	CB	ASP	755		-10.584	30.628	1.00 49.89
ATOM	6002	CG	ASP	755		-11.616	30.717	1.00 51.73
ATOM	6003	OD1		755		-11.680	31.785	1.00 55.47
ATOM	6004	OD2		755		-12.354	29.738	1.00 50.98
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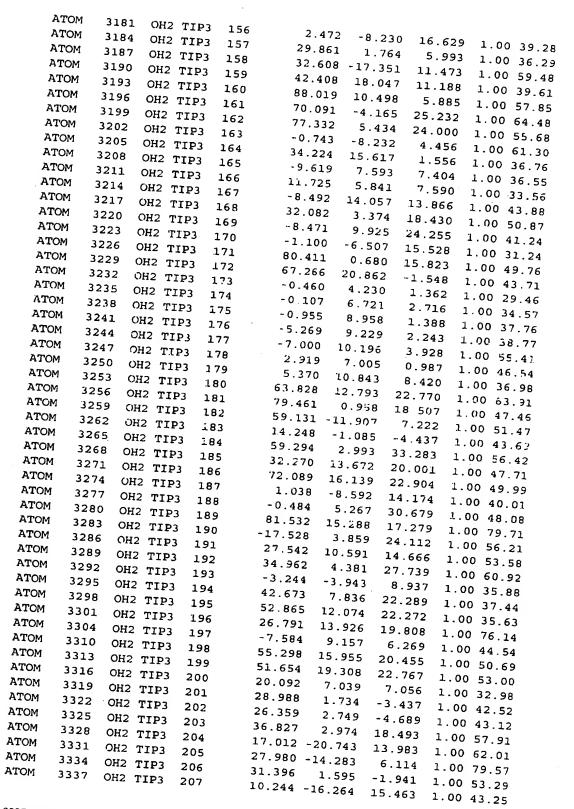
<b>&gt;-</b>	
ATOM 6005 C ASP 7	55 56 024
710M 6006 0 ACD 7	
ALOM 6007 N ARC TO	36.021 -13.107 29 155
ATOM 6009 CA ARG 75	33.22/ -11.940 30 917
ATOM 6010 CB ARG 75	34.332 -12.989 31 395
ATOM 6011 CG ARG 75	53.556 -12.501 32 611 3 05
ATOM 6012 CD 375	52.389 -13.380 33 029 1 22
ATOM 6013 NE APC	51.672 -12.772 34 215 7 34.26
ATOM 6015 CZ ARC 35	51.293 -11.382 33 969 1 00 56.76
ATOM 6016 NH1 ARC	50.259 -11.002 33 221
ATOM 6019 NUL 750	49.487 -13 000 2.00 62.60
ATOM 6022 C	49.986
ATOM 6023 0 700	53.357 -13 420 1.00 63.72
ATOM 6024 N 775	53.243 -14 507
ATOM 6026 CD 757	52.687 -12 452 1.00 54.82
ATOM 6022	51.709 -12 722 1.00 51.18
ATOM COOK THE 757	53 005
20020 CG2 ILE 757	50 712 28.120 1.00 47 88
Amove CGI ILE 757	50 242 26.953 1.00 45 56
CDI ILE 752	49.653 29.258 1.00 47 77
ATOM SORE LLE 757	52 224 28.914 1.00 46 00
ATOM COST	51 604 27.449 1.00 48 30
ATOM 555 758	53 522 26.937 1.00 45 63
Amore CA VAL 758	54 303 "5 27.038 1.00 48 88
758 VAL 758	55 602 25.912 1.00 49 96
Amon 6037 CG1 VAL 758	
758 CG2 VAL 758	36.313 -13.864 24 502
ATOM 6039 C VAL 758	33.461 -11.660 25 190
ATOM 6040 O VAL 750	
ATOM 6041 N ALA 759	34.218 -16.050 25 206
A10M 6043 CA ALA 759	34.69/ -15.540 27 445
0044 CB ALA 750	34.898 ·16.926 27 R44
MO11 6045 C ALA 759	33.44/ -16.987 29 252 4 25
A10M 6046 O ALA 750	33.592 -17.702 27 761 1 62.30
ATOM 6047 N LEU 760	53.555 -18.823 27 254 3 35
ATOM 6049 CA LEU 760	52.519 -17.090 28 248
ATOM 6050 CB LEU 760	31.20917.720 28 245 3 45
ATOM 6051 CG LEU 760	50.314 -17.090 29 320 1 00
ATOM 6052 CD1 TEXT	50.729 -17.330 30 777 1 22
ATOM 6053 CD2 TEG	49.808 -16.563 31 722 1 00 67.01
ATOM 6054 C LETT 755	30.701 -18.819 31 083
6055 O LEU 760	50.510 -17.666 26 882 1 55.17
ATOM 6056 N TUD	49.342 -18.039 26 707 1.19
ATOM 6058 CA TUD	51.210 -17.201 25 860 1 00 /3.15
ATOM 6059 CB THE	50.626 -17.113 24 518 7 3.38
ATOM 6060 OCT TOTAL	50.963 -15.760 23 820 1 5
ATOM 6062 CC2	50.353 -14 600
ATOM 6063 C	50.435 15 72
ATOM 5064 0 THR 761	51.080 -10 276 7.00 /0.32
ATOM 6005 THR 761	52.276 -19 500
ATOM 6066 CC 1603	19.100 0.00
ATOM 6067 CD MET 534	69.385 13.205 19.903 0.50 30.84 PRT2
ATOM 6060 TO MET 534	69.112 13 220 - 45.593 0.50 33.69 PRT2
6068 CE MET 534	70.067 12 420 - 0.50 34.44 PRT2
	70.067 12.429 26.060 0.50 36.92 PRT2
CCCD /	- ***2

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ATOM	6069	SG	CYS	603	56.370	-7.959	16.451	0.50 41.20 I	PRT2
ATOM	2716	OH2	TIP3	1	71.864	25.128	2.721	1.00 26.20	
ATOM	2719	OH2	TIP3	2	39.862	4.160	16.115	1.00 42.43	
ATOM	2722	OH2	TIP3	3	83.875	19.969	10.572	1.00 23.41	
ATOM	2725	OH2	TIP3	4	83.585	20.356	7.953	1.00 30.15	
ATOM	2728	OH2	TIP3	5	75.100	16.407	6.948	1.00 46.78	
ATOM	2731	OH2	TIP3	6	86.616	19.701	9.707	1.00 44.37	
ATOM	2734	OH2	TIP3	7	52.270	10.726	24.472	1.00 40.13	
ATOM	2737			8	55.346	9.394	22.489	1.00 29.09	
ATOM	2740	OH2	TIP3	9	56.794	4.380	32.527	1.00 28.02	
ATOM	2743	OH2	TIP3	10	52.425	4.653	13.421	1.00 18.63	
ATOM	2746	OH2	TIP3	11	41.527	5.347	22.682	1.00 32.60	
ATOM	2749	OH2	TIP3	12	44.868	9.058	21.659	1.00 34.90	
ATOM	2752	ОН2	TIP3	13	64.548	-2.881	29.048	1.00 32.56	
ATOM	2755	ОН2	TIP3	14	77.179	13.205	23.892	1.00 30.36	
ATOM	2758	ОН2	TIP3	15	79.309	16.826	18.132	1.00 55.69	
ATOM	2761		TIP3	16	83.279	11.681	16.069	1.00 21.18	
MOTA	2764		TIP3	17	13.978	-9.614	0.374	1.00 23.81	
MOTA	2767		TIP3	18	38.294	0.616	5.237	1.00 48.89	
ATOM	2770		TIP3	19	27.114	6.248	5.051	1.00 19.82	
ATOM	2773		TIP3	20	34.369	-1.759		1.00 43.83	
ATOM	2776			21	20.500	2.296	28.237	1.00 53.46	
ATOM	2779		TIP3	22		-11.733	38.257	1.00 51.73	
ATOM	2782		TIP3	23	17.066	-5.917	-2.027	1.00 29.88	
ATOM	2785	OH2	TIP3	24	27.873	8.078	15.136	1.00 45.40	
ATOM	2788		TIP3	25	31.459	0.037	6.873	1.00 33.38	
ATOM	2791		TIP3	26		-12.845	27.724	1.00 37.01	
MOTA	2794		TIP3	27		-17.329	12.884	1.00 37.31	
MOTA	2797	ОН2	TIP3	28	88.863	14.111	8.054	1.00 41.25	
ATOM	2800		TIP3	29 .	-2.311	-3.712	11.483	1.00 30.72	
MOTA	2803	OH2	TIP3	30	34.895	.4.269	18.658	1.00 28.99	
MOTA	2806		TIP3	31	80.531	18.007	9.739	1.00 23.83	
ATOM	2809	OH2	TIP3	32	5.519	3.787	10.628	1.00 20.39	
ATOM	2812	OH2	TIP3	33	-10.523	5.304	11.469	1.00 20.31	
ATOM	2815	OH2	TIP3	34	29.538	-8.848	20.187	1.00 43.26	
ATOM	2818		TIP3	35	5.866	3.469	13.367	1.00 21.16	
ATOM	2821	OH2	TIP3	36	31.810	3.038	0.203	1.00 65.03	
ATOM	2824	OH2	TIP3	37	19.879	2.087	-3.828	1.00 34.62	
MOTA	2827	OH2	TIP3	38	61.882	2.577	32.790	1.00 43.01	
ATOM	2830		TIP3	39	21.062	-6.897	-4.255	1.00 26.18	
ATOM	2833	OH2	TIP3	40	-15.562	8.847	22.744	1.00 40.33	
ATOM	2836	OH2	TIP3	41	40.043	2.380	8.610	1.00 65.14	
ATOM	2839		TIP3	42	19.176	11.322	0.332	1.00 33.04	
ATOM	2842		TIP3	43	67.221	8.965	17.535	1.00 14.78	
ATOM	2845		TIP3	44	87.877	18.828	18.789	1.00 50.00	
MOTA	2848		TIP3	45	74.676	17.083	4.253	1.00 43.45	
MOTA	2851		TIP3	46	29.458	16.709	10.527	1.00 37.44	
ATOM	2854		TIP3	47	66.590	7.242	15.359	1.00 27.63	
ATOM	2857		TIP3	48	85.038	21.651	5.881	1.00 27.12	
ATOM	2860		TIP3	49	-4.762	3.091	3.313	1.00 13.83	
ATOM	2863		TIP3	50	19.509	4.951	5.063	1.00 33.74	
ATOM	2866		TIP3	51	34.833	5.465	24.635	1.00 33.74	
		Ţ				105			

A TOLE		
ATOM 2869 OH2 TI	P3 52	2 24 222
AIUM 2872 OH2 TOT	P3 53	34.907 ~17.187 13.739 1.00 28
ALUM 2875 OH2 TT	-	7.568 27 992 "
ATOM 2878 OH2 TI		-7.341 -1.418 6 300 1.00 31.38
ATOM 2881 OH2 TI		55.218 12 161
A MON	56	68.597
ATION	P3 57	73.486 20.953 1.00 45.39
ATTOM -	93 58	3 555 19.260 1.00 49 23
ATTOM	93 59	38 079 10 -8.166 1.00 20 02
AMON.	93 60	29 917 5.669 1.00 27 07
AMON.	9 61	-1.649 7 00 44 22
ATOM 2899 OH2 TIP	3 62	12.262 1 00 42 70
ATOM 2902 OH2 TID	3 63	3.969 28.834 1 00 27
ATOM 2905 OH2 TIP	_	10.523 -13.468 0 964
AIUM 2908 OH2 TITE		-1,001
ATOM -	_	30.278 15 425 27 27 27 35.58
ATOM 2014		8.115 4.204 1.00 48.75
ATOM CONTRACT ON THE		73 460 3.317 1.00 16 04
ATOM	68	-P 043 - 42.744 1.00 34 70
ATOM	69	24.939 1 00 44 05
One Tips	70	
2926 OH2 TIP3	71	21.//0 -20.943 4.990 1.00 32.39
A10M 2929 OH2 TIDE	72	39.587 -6.482 5.010
ATOM 2932 OH2 TITES		16.676 -13.158 -2 022
410M 2935 OH2 TIDE	73	-15.177 7.529 4 524
ATOM 2938 OH2 TIP3	74	33.105
7004	75	0.334 205 1.00 40.43
Machine and Outs 1153	76	17.489 2 560 - 1.00 31.20
NTO 0112 11P3	77	27 272 2.500 3.445 1.00 16 38
7.TOM	78	-8 546 6 5 5 6 1.00 39 52
Amon OH2 TIF3	79	- 9.673 1 00 17 00
Amore Onz Tip3	80	8,809 7 00 33
ATOM 2956 OH2 TIP3	91	-4.985 -3.024 6.965 1.00 30.55
ATOM 2959 OH2 TTD	82	17.673 3.019 1.736
ATOM 2962 OH2 TITE		20.319 3.536 2 993
2965 OH2 TTD2	83	0.366 -2.419 22 242 1 20 20.39
A10M 2968 OH2 TITE	84	19.688 -6.134 -1.678
ATOM 2971 OH2 TIP3	85	10.581 -15 492
ATOM - TIES	86	4.476 -12 260 - 1.09 43.14
70014	87	6.421 1.053
ATTOM	88	-13 766 -3.368 1.00 21.50
ACCOM DH2 TIP3	89	15 600 5.565 1.00 39 45
ONZ 110{	90	-0.140 1 00 30 55
ATOM	91	3.937 1 00 21
ATOM 2989 OH2 TIP3	92	-4.424 1 00 25 -
2992 OH2 TIP3	93	2,309 7 00 44
2995 OH2 TIP3	94	24.342 -13.465 -0.010 7 00 50 7
ATOM 2998 OH2 TID2		00.334 -4.675 33 970
ATOM 3001 OVE	95	10.408 5.632 3.429
ATOM 3004 OVID	96	-9.676 -3.036
ATOM 3007 OVA	97	73.207 -2 075
Amore Onz 11P3	98	-3.042 5.407 1.00 70.04
ATTOM	99	36 627 0 202 1.00 30.78
ATTOM 3013 OH2 TIP3 10		21 605 1.645 1.00 41 40
ATOM 3016 OH2 TIP3 10	_	21.085 6.318 16.814 1.00 20 93
3019 OH2 TTD2		0.662 19.231 1 00 57 22
ATOM 3022 OH2 TIP3 10		3.793 -8.713 22.177 1 00 54 77
22 3 10	-	-13.037
SCOP II		6.412 17.695 1.00 25.61
SSSD/55145 01		

ATOM	3025	OH2 TIP3	104	26.597	-10.647	-1.184	1.00	25.85
MOTA	3028	OH2 TIP3	105	24.406	1.951	18.037	1.00	30.72
ATOM	3031	OH2 TIP3	106	-1.809	12.914	3.754	1.00	43.57
ATOM	3034	OH2 TIP3	107	59.590	13.738	33.131	1.00	26.96
ATOM	3037	OH2 TIP3	108	4.442	-11.011	1.724	1.00	46.96
MOTA	3040	OH2 TIP3	109	8.101	2.869	0.801	1.00	37.28
MOTA	3043	OH2 TIP3	110	76.065	1.631	26.158	1.00	46.49
ATOM	3046	OH2 TIP3	111	48.821	15.839	14.239	1.00	34.18
ATOM	3049	OH2 TIP3	112	2.703	-11.324	8.959	1.00	39.16
MOTA	3052	OH2 TIP3	113	82.922	26.478	12.953	1.00	43.77
ATOM	3055	OH2 TIP3	114	8.998	-6.359	-3.309	1.00	39.51
ATOM	3058	OH2 TIP3	115	-8.590	4.563	4.397	1.00	32.53
ATOM	3061	OH2 TIP3	116	8.115	-13.800	8.351	1.00	41.64
MOTA	3064	OH2 TIP3	117	51.643	6.187	10.821	1.00	31.70
MOTA	3067	OH2 TIP3	118	20.737	3.915	15.522	1.00	17.40
ATOM	3070	OH2 TIP3	119	73.254	3.698	20.947	1.00	27.49
ATOM	3073	OH2 TIP3	120	5.343	-11.780	22.588	1.00	36.63
MOTA	3076	OH2 TIP3	121	34.390	2.307	16.660	1.00	64.04
MOTA	3079	OH2 TIP3	122	9.552	-11.846	6.934	1.00	28.23
ATOM	3082	OH2 TIP3	123	8.463	4.098	-1.454	1.00	30.21
MOTA	3085	OH2 TIP3	124	7.397	6.952	2.826	1.00	33.87
MOTA	3088	OH2 TIP3	125	35.796	-1.428	0.072	1.00	30.27
ATOM	3091	OH2 TIP3	126	45.044	10.052	11.102	1.00	28.75
ATOM	3094	OH2 TIP3	127	45.209	11.756	21.279	1.00	31.80
ATOM	3097	OH2 TIP3	128	-2.800	15.170	16.902	1.00	32.72
ATOM	3100	OH2 TIP3	129	85.885	11.248	9.428	T.00	25.28
ATOM	3103	OH2 TIP3	130	13.136	-2.420	1.867	1.00	20.56
ATOM	3106	OH2 TIP3	131	75.900.	3.542	20.641	1.00	39.79
ATOM	3109	OH2 TIP3	132	13.075	7.580	-2.817	1.00	34.49
MOTA	3112	OH2 TIP3	133	11.166	-10.189	0.573	1.00	36.71
ATOM	3115	OH2 TIP3	134		-16.459	3.327	1.00	21.18
MOTA	3118	OH2 TIP3	135	-6.419	-3.460	16.599		32.62
ATOM	3121	OH2 TIP3	136		-12.834	3.624		43.32
ATOM	3124	OH2 TIP3	137	-16.472	11.136	6.388		64.77
MOTA	3127	OH2 TIP3	138	86.531	12.711	7.151		28.72
ATOM	3130	OH2 TIP3	139	32.292	-4.665	1.511		30.98
ATOM	3133	OH2 TIP3	140	45.116	7.369	11.774		30.59
ATOM	3136	OH2 TIP3	141	81.035	12.317	16.907		41.72
ATOM	3139	OH2 TIP3	142	2.905	-7.019	-2.101		26.20
ATOM	3142	OH2 TIP3	143	31.895	-6.253	20.885		36,12
ATOM	3145	OH2 TIP3	144	74.974	-2.640	12.464		58.90
ATOM	3148	OH2 TIP3	145	7.514	6.734	-1.116		37.81
ATOM	3151	OH2 TIP3	146	71.606	5.595	22.198	1.00	
ATOM	3154	OH2 TIP3	147	68.337	-5.037	8.955	1.00	
ATOM	3157	OH2 TIP3	148	0.191	-9.669	6.903	1.00	
ATOM	3160	OH2 TIP3	149	68.043	18.153	10.710	1.00	
ATOM	3163	OH2 TIP3	150	3.644	8.512	4.478	1.00	
ATOM	3166	OH2 TIP3	151	52.117	11.302	18.644	1.00	
MOTA	3169	OH2 TIP3	152	-10.220	6.750	4.981	1.00	
ATOM	3172	OH2 TIP3	153	76.944	1.425	-0.793	1.00	
ATOM	3175	OH2 TIP3	154		-11.958	17.014	1.00	
ATOM	3178	OH2 TIP3	155	34.348	14.128	18.169	1.00	42.98





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ATOM	3340	OH2	TIP3	208	7.25	5 -11.909	5.440	1.00	45.52
MOTA	3343	OH2	TIP3	209	-12.42	L 14.520	11.103	1.00	56.32
ATOM	3346	OH2	TIP3	210	11.250	9.879	-1.498	1.00	28.34
MOTA	3349	OH2	TIP3	211	11.426	12.574	-1.341	1.00	37.79
ATOM	3352	OH2	TIP3	212	34.344	13.104	-1.291	1.00	51.83
ATOM	3355	OH2	TIP3	213	31.230	18.082	8.054	1.00	44.77
ATOM	3358	OH2	TIP3	214	37.062	12.036	-1.875	1.00	53.61
MOTA	3361	OH2	TIP3	215	. 35.231	3.150	10.692	1.00	60.59
ATOM	3364	OH2	TIP3	216	63.913	13:371	26.770	1.00	59.44
ATOM	3367	OH2	TIP3	217	36.511	6.165	15.409	1.00	70.98
ATOM	3370	OH2	TIP3	218	90.623	4.459	6.671		52.23
ATOM	3373	OH2	TIP3	219	49.822	-11.758	10.881		46.12
ATOM	3376	OH2	TIP3	220	60.367	-10.286	16.662		68.41
ATOM	3379	OH2	TIP3	221	17.954	-21.378	7.048		68.51
ATOM	3382	OH2	TIP3	222	66.176		30.784		39.19
MOTA	3385	OH2	TIP3	223	75.201		20.800		43.98
ATOM	3388	OH2	TIP3	224	-2.895		3.534		44.97
MOTA	3391	OH2	TIP3		6.045		25.279		63.74
ATOM	3394	OH2	TIP3		36.238		12.819		32.89
ATOM	3397	OH2	TIP3	227	-5.516		14.089		51.60
ATOM	3400	OH2			46.577		26.964		37.76
ATOM	3403	OH2	TIP3		6.496		13.722		27.51
ATOM	3406	OH2	TIP3		-3.691		20.691		38.16
MOTA	3409	OH2	TIP3	231	1.811		-0.149		54.03
ATOM	3412	OH2	TIP3	232	86.148		23.402		57.66
MOTA	3415	OH2	TIP3	233	10.549		5.716		48.49
MOTA	3421	OH2	TIP3	234	64.680		20.697		69.67
ATOM	3424	OH2	TIP3	235	11.380		13.500	1.00	54.61
ATOM	3427	OH2	TIP3	236	3.136		21.980		57.12
MOTA	3430	OH2	TIP3	23.7	72.296		-1.987		41.40
MOTA	3433	OH2	TIP3	238	50.258		32.723		74.99
MOTA	3436	OH2	TIP3	239	58.051		11.776		44.10
MOTA	3439	OH2	TIP3	240	43.530	20.498	30.344		43.69
MOTA	3442	OH2	TIP3	241	67.081	16.597	15.934	1.00	45.80
ATOM	3445	OH2	TIP3	242	87.660	21.694	5.373		59.39
ATOM	3448	OH2	TIP3	243	71.779	28.586	7.932		61.12
ATOM	3451	OH2	TIP3	244	25.965	-8.124	27.084		42.13
MOTA	3454	OH2	TIP3	245	-18.336	10.487	12.859		73.36
MOTA	3457	OH2	TIP3	246	30.703	11.410	16.381	1.00	39.24
MOTA	3460	OH2	TIP3	247		-16.025	-2.906	1.00	63.22
ATOM	4620	С	SUG	1000	67.815	4.441	11.493		20.00
MOT'A	4621	C1	SUG	1000	67.387	3.706	10.364		20.00
ATOM	4622	N	SUG	1000	67.823	2.445	9.937		20.00
MOTA	4623	C2	SUG	1000	66.401	4.224	9.501		20.00
MOTA	4624	C3	SUG	1000	65.825	5.499	9.765		20.00
ATOM	4625	C4	SUG	1000	66.259	6.212	10.884	1.00	
MOTA	4626	C5	SUG	1000	67.239	5.690	11.736	1.00	
ATOM	4627	C6	SUG	1000	66.155	3.220	8.401	1.00	
ATOM	4628	0	SUG	1000	67.372	1.047	8.275	1.00	
MOTA	4629	C7	SUG	1000	67.155	2.121	8.828	1.00	
ATOM	4630	C8	SUG	1000	63.369	2.460	5.852	1.00	
ATOM	4631	C9	SUG	1000	65.284	3.356	7.382	1.00	

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TABLE 4

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Atom No. Type Type No. No. No. No. Type No.		V	Y	z oc	CC B
No.    Type   Type   No.   No.   17.066   8.598   1.00   57.39     ATOM   1 N   GLU   1464   -11.3576   17.066   8.598   1.00   57.39     ATOM   3 CB   GLU   1464   -11.381   18.127   7.684   1.00   55.07     ATOM   4 C   GLU   1464   -11.81   15.833   7.341   1.00   55.07     ATOM   5 O   GLU   1464   -11.722   15.504   6.165   1.00   59.74     ATOM   6 N   LEU   1465   -10.550   13.699   8.347   1.00   40.50.12     ATOM   7 CA   LEU   1465   -10.550   13.3699   9.291   1.00   43.28     ATOM   9 CG   LEU   1465   -8.630   13.316   9.291   1.00   43.28     ATOM   10   CD1   LEU   1465   -8.630   13.316   9.291   1.00   43.70     ATOM   10   CD1   LEU   1465   -8.630   13.316   9.291   1.00   43.70     ATOM   11   CD2   LEU   1465   -8.022   14.754   9.013   1.00   47.59     ATOM   12   C   LEU   1465   -12.046   12.697   7.739   1.00   40.93     ATOM   13   O   LEU   1465   -13.139   12.730   8.301   1.00   39.13     ATOM   14   N   PRO   1466   -11.794   11.852   6.726   1.00   40.49     ATOM   16   CA   PRO   1466   -12.754   10.831   6.284   1.00   40.94     ATOM   16   CA   PRO   1466   -12.152   10.331   4.991   1.00   40.94     ATOM   18   CG   PRO   1466   -12.152   10.331   4.991   1.00   40.94     ATOM   19   C   PRO   1466   -12.152   10.331   4.991   1.00   40.94     ATOM   20   O   PRO   1466   -12.166   -10.664   10.518   6.284   1.00   40.94     ATOM   21   N   GLU   1467   -14.664   -15.728   8.054   8.467   1.00   39.07     ATOM   22   CA   GLU   1467   -14.664   -15.728   8.054   8.677   7.891   1.00   40.95     ATOM   23   CB   GLU   1467   -16.314   9.365   9.353   1.00   50.91     ATOM   24   CG   GLU   1467   -18.379   9.252   9.699   1.00   53.51     ATOM   25   CD   GLU   1467   -18.379   9.252   9.699   1.00   53.51     ATOM   32   CB   ASP   1468   -12.750   3.065   3.00   3.07     ATOM   33   CA   ASP   1468   -12.750   3.065   3.00   3.07     ATOM   34   CD   PRO   1469   -14.063   3.019   9.305   1.00   25.83     ATOM   35   OA   SP   1468   -12.570   3.065   3.00   3.00   3.00     A	A t OM		_		
ATOM         1         N         GLU         1464         -12.446         17.198         7.684         1.00         55.73           ATOM         2         CA         GLU         1464         -11.381         18.127         8.275         1.00         55.73           ATOM         4         C         GLU         1464         -11.191         15.833         7.341         1.00         55.73           ATOM         5         O         GLU         1465         -11.518         15.034         8.347         1.00         59.74           ATOM         6         N         LEU         1465         -10.950         13.699         8.087         1.00         43.28           ATOM         9         CG         LEU         1465         -10.155         13.199         9.291         1.00         43.28           ATOM         11         CD2         LEU         1465         -10.155         13.139         9.227         1.00         43.28           ATOM         13         LEU         1465         -12.046         12.697         7.739         1.00         40.90           ATOM         15         CD         PRO         1466         -12.046		Type Type No.	17.066	8.598 1	.00 57.39
ATOM 3 CB GLU 1464 -11.381 18.127 7.341 1.00 55.07 ATOM 4 C GLU 1464 -11.381 18.127 7.341 1.00 55.07 ATOM 4 C GLU 1464 -11.722 15.504 6.165 1.00 59.74 ATOM 5 O GLU 1465 -10.950 13.699 8.087 1.00 44.43 ATOM 7 CA LEU 1465 -10.950 13.699 9.291 1.00 43.28 ATOM 8 CB LEU 1465 -10.950 13.196 9.291 1.00 43.28 ATOM 9 CG LEU 1465 -8.222 14.754 9.013 1.00 47.59 ATOM 10 CD1 LEU 1465 -8.630 13.316 9.227 1.00 43.70 ATOM 11 CD2 LEU 1465 -8.222 14.754 9.013 1.00 47.59 ATOM 12 C LEU 1465 -13.139 12.730 8.301 1.00 39.13 ATOM 13 O LEU 1465 -13.139 12.730 8.301 1.00 39.13 ATOM 15 CD PRO 1466 -11.794 11.852 6.726 1.00 40.93 ATOM 15 CD PRO 1466 -10.612 11.884 1.00 39.07 ATOM 16 CA PRO 1466 -10.612 11.884 1.00 39.07 ATOM 19 C PRO 1466 -10.664 10.518 5.202 1.00 40.94 ATOM 19 C PRO 1466 -10.664 10.518 5.202 1.00 40.90 ATOM 19 C PRO 1466 -10.664 10.518 5.202 1.00 40.90 ATOM 20 O PRO 1466 -10.664 10.518 5.202 1.00 40.90 ATOM 20 O PRO 1466 -10.664 10.518 5.202 1.00 40.90 ATOM 20 C B GLU 1467 -14.255 8.126 8.467 1.00 39.43 ATOM 20 C B GLU 1467 -14.255 8.126 8.467 1.00 39.13 ATOM 20 C G GLU 1467 -14.255 8.126 8.467 1.00 39.24 ATOM 20 C G GLU 1467 -18.369 10.250 10.050 ATOM 20 C G GLU 1467 -18.369 10.250 10.050 ATOM 20 C G GLU 1467 -18.369 10.250 10.050 ATOM 20 C G GLU 1467 -18.369 10.250 ATOM 20 C ASP 1468 ATOM 31 CA ASP 1468 ATOM 32 CB ASP 1468 ATOM 33 CA ASP 1468 ATOM 34 ODL ASP 1468 ATOM 35 ODZ ASP 1468 ATOM 35 ODZ ASP 1468 ATOM 37 O ASP 1468 ATOM 38 N PRO 1469 ATOM 40 CA		1 N GLU 1464 -13.376	17.198	7.684 1	.00 55.83
ATOM		- Gr CIII 1464 -12.440	18 127	8.275 1	.00 56.73
ATOM		3 CB GLU 1464 -11.381	15 833	7 341 1	.00 55.07
ATOM 6 N LEU 1465 -11.518 15.023 8.347 1.00 50.12 ATOM 6 N LEU 1465 -10.155 13.699 8.087 1.00 44.43 ATOM 7 CA LEU 1465 -10.155 13.196 9.291 1.00 43.28 ATOM 9 CG LEU 1465 -8.630 13.316 9.227 1.00 43.70 ATOM 10 CD1 LEU 1465 -8.630 13.316 9.291 1.00 47.59 ATOM 11 CD2 LEU 1465 -8.222 14.754 9.013 1.00 47.59 ATOM 12 C LEU 1465 -12.046 12.697 7.739 1.00 40.93 ATOM 13 O LEU 1465 -13.139 12.730 8.301 1.00 39.13 ATOM 14 N PRO 1466 -12.046 11.892 6.726 1.00 40.49 ATOM 15 CD PRO 1466 -12.754 10.831 4.981 1.00 40.90 ATOM 17 CB PRO 1466 -12.152 10.331 4.981 1.00 40.14 ATOM 16 CA PRO 1466 -12.862 9.701 7.305 1.00 40.90 ATOM 19 C PRO 1466 -12.862 9.701 7.305 1.00 40.06 ATOM 20 O PRO 1466 -12.862 9.701 7.305 1.00 40.06 ATOM 21 N GLU 1467 -14.654 9.175 7.491 1.00 38.65 ATOM 22 CA GLU 1467 -14.255 8.126 8.647 1.00 39.24 ATOM 23 CB GLU 1467 -15.722 8.054 8.873 1.00 40.06 ATOM 24 CG GLU 1467 -16.314 9.365 9.591 ATOM 25 CD GLU 1467 -17.789 9.252 9.699 1.00 53.51 ATOM 27 OEZ GLU 1467 -17.789 9.252 9.699 1.00 53.51 ATOM 28 C GLU 1467 -18.379 8.170 9.504 1.00 54.15 ATOM 29 O GLU 1467 -18.369 10.250 10.160 1.00 53.10 ATOM 27 OEZ GLU 1467 -13.922 6.529 8.407 1.00 38.58 ATOM 30 N ASP 1468 -13.272 5.929 8.407 1.00 28.23 ATOM 31 CA ASP 1468 -13.272 5.929 8.407 1.00 28.23 ATOM 32 CB ASP 1468 -13.274 3.527 5.929 8.791 1.00 27.68 ATOM 33 CG ASP 1468 -13.274 3.527 5.929 8.791 1.00 27.68 ATOM 34 OD1 ASP 1468 -13.274 3.627 9.930 1.00 25.51 ATOM 37 O ASP 1468 -13.274 3.627 9.930 1.00 25.88 ATOM 36 C ASP 1468 -13.274 3.627 9.930 1.00 27.74 ATOM 37 O ASP 1468 -12.570 3.186 9.941 1.00 24.25 ATOM 38 N PRO 1469 -15.396 3.175 9.935 1.00 27.74 ATOM 40 CA PRO 1469 -14.963 2.079 9.930 1.00 27.74 ATOM 41 CB PRO 1469 -14.963 2.079 9.305 1.00 27.74 ATOM 42 CG PRO 1469 -14.963 2.079 9.305 1.00 27.74 ATOM 40 CA PRO 1469 -14.963 2.079 9.305 1.00 27.74 ATOM 40 O PRO 1469 -14.910 0.925 10.625 1.00 27.74 ATOM 41 CB PRO 1469 -14.910 0.925 10.625 1.00 27.50		4 C GLU 1464 "11.843	15.504	6 165 1	.00 59.74
ATOM 6 N LEU 1465		5 O GLU 1464 -11.722	15.023	8 347 1	00 50.12
ATOM 8 CB LEU 1465 -10.930		TIT 1465		a 087 1	.00 44.43
ATOM 9 CG LEU 1465 ATOM 10 CD1 LEU 1465 ATOM 11 CD2 LEU 1465 ATOM 12 C LEU 1465 ATOM 13 O LEU 1465 ATOM 14 N PRO 1466 ATOM 15 CD PRO 1466 ATOM 16 CA PRO 1466 ATOM 17 CB PRO 1466 ATOM 18 CG PRO 1466 ATOM 19 C PRO 1466 ATOM 19 C PRO 1466 ATOM 20 O PRO 1466 ATOM 21 N GLU 1467 ATOM 21 N GLU 1467 ATOM 23 CB GLU 1467 ATOM 24 CG GLU 1467 ATOM 25 CD GLU 1467 ATOM 26 OEI GLU 1467 ATOM 27 OE2 GLU 1467 ATOM 27 OE2 GLU 1467 ATOM 28 C GLU 1467 ATOM 29 O GLU 1467 ATOM 26 OEI GLU 1467 ATOM 27 OE2 GLU 1467 ATOM 28 C GLU 1467 ATOM 29 O GLU 1467 ATOM 29 O GLU 1467 ATOM 26 OEI GLU 1467 ATOM 27 OE2 GLU 1467 ATOM 28 C GLU 1467 ATOM 29 O GLU 1467 ATOM 29 O GLU 1467 ATOM 30 N ASP 1468 ATOM 31 CA ASP 1468 ATOM 32 CB ASP 1468 ATOM 33 CG ASP 1468 ATOM 34 ODI ASP 1468 ATOM 35 OD2 ASP 1468 ATOM 36 C ASP 1468 ATOM 37 O ASP 1468 ATOM 38 N PRO 1469 ATOM 38 N PRO 1469 ATOM 39 CD PRO 1469 ATOM 40 CA PRO 1469 ATOM 40 CA PRO 1469 ATOM 41 CB PRO 1469 ATOM 41 CB PRO 1469 ATOM 42 CG PRO 1469 ATOM 44 O PRO 1469 ATOM 45 N ARG 1470 ATOM 46 O PRO 1469 ATOM 47 O PRO 1469 ATOM 48 O PRO 1469 ATOM 49 O PRO 1469 ATOM 40 CR PRO 1469 ATOM		7 CA LEU 1465		9.291	.00 43.28
ATOM 10 CD1 LEU 1465 -8.032 14.754 10.506 1.00 47.59   ATOM 11 CD2 LEU 1465 -8.222 14.754 10.506 1.00 42.63   ATOM 12 C LEU 1465 -12.045 12.803 10.506 1.00 42.63   ATOM 13 O LEU 1465 -13.139 12.730 8.301 1.00 40.93   ATOM 14 N PRO 1466 -13.139 12.730 8.301 1.00 39.13   ATOM 15 CD PRO 1466 -10.612 11.884 5.844 1.00 39.07   ATOM 16 CA PRO 1466 -12.754 10.831 6.284 1.00 40.14   ATOM 17 CB PRO 1466 -12.754 10.831 6.284 1.00 40.14   ATOM 18 CG PRO 1466 -12.152 10.331 4.991 1.00 40.90   ATOM 19 C PRO 1466 -12.862 9.701 7.305 1.00 40.06   ATOM 20 O PRO 1466 -11.857 9.290 7.883 1.00 40.71   ATOM 21 N GLU 1467 -14.255 8.126 8.467 1.00 39.24   ATOM 22 CA GLU 1467 -14.255 8.126 8.467 1.00 39.24   ATOM 24 CG GLU 1467 -14.255 8.126 8.467 1.00 39.24   ATOM 25 CD GLU 1467 -16.314 9.365 9.353 1.00 50.91   ATOM 26 OEI GLU 1467 -17.789 9.252 9.699 1.00 53.51   ATOM 27 OE2 GLU 1467 -18.379 9.252 9.699 1.00 53.51   ATOM 28 C GLU 1467 -18.369 10.250 10.160 1.00 36.09   ATOM 30 N ASP 1468 -13.272 8.954 1.00 30.71   ATOM 31 CA ASP 1468 -10.885 3.207 7.592 1.00 25.51   ATOM 32 CB ASP 1468 -10.885 3.207 7.592 1.00 25.51   ATOM 34 ODI ASP 1468 -11.623 -12.570 3.405   ATOM 35 OD2 ASP 1468 -13.272 3.627 7.529 1.00 25.88   ATOM 36 C ASP 1468 -12.570 3.405   ATOM 37 O ASP 1468 -12.570 3.405   ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88   ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 25.88   ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 25.88   ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 25.88   ATOM 41 CB PRO 1469 -14.450 3.019 9.305 1.00 25.88   ATOM 41 CB PRO 1469 -14.450 3.019 9.305 1.00 25.88   ATOM 41 CB PRO 1469 -14.450 3.019 9.305 1.00 27.76   ATOM 44 O PRO 1469 -14.450 3.019 9.305 1.00 27.76   ATOM 44 O PRO 1469 -14.4102 0.925 10.625 1.00 27.50   ATOM 44 O PRO 1469 -14.4102 0.925 10.625 1.00 27.50   ATOM 44 O PRO 1469 -14.4102 0.925 10.625 1.00 27.50   ATOM 44 O PRO 1469 -14.4102 0.925 10.625 1.00 27.60   ATOM 44 O PRO 1469 -14.4102 0.925 10.625 1.00 27.60   ATOM 45 N ARG 1470 -14.100 -14.100 -14.100 -14.100   ATOM 44 O PRO 146		8 CB LEU 1465 -10.155		9.227	1.00 43.70
ATOM 10 CD1 LEU 1465 -8.22		70 TEIL 1465 -8.630		9.013	1.00 47.59
ATOM 12 C2 LEU 1465 -8.04 12.697 7.739 1.00 40.93 ATOM 12 C LEU 1465 -12.046 12.697 7.739 1.00 40.93 ATOM 13 O LEU 1465 -12.016 12.697 7.739 1.00 40.49 ATOM 14 N PRO 1466 -11.794 11.852 6.726 1.00 40.49 ATOM 15 CD PRO 1466 -10.612 11.884 5.844 1.00 39.07 ATOM 16 CA PRO 1466 -12.754 10.831 4.981 1.00 40.90 ATOM 17 CB PRO 1466 -12.862 9.701 7.305 1.00 40.06 ATOM 18 CG PRO 1466 -12.862 9.701 7.305 1.00 40.06 ATOM 19 C PRO 1466 -14.064 9.175 7.491 1.00 38.65 ATOM 22 CA GLU 1467 -14.064 9.175 ATOM 23 CB GLU 1467 ATOM 24 CG GLU 1467 -16.314 9.365 9.353 1.00 50.91 ATOM 27 OEZ GLU 1467 ATOM 26 OEL GLU 1467 -17.789 9.252 9.699 1.00 53.51 ATOM 29 O GLU 1467 -18.379 8.170 ATOM 29 O GLU 1467 -18.379 8.170 ATOM 29 O GLU 1467 -18.369 6.777 ATOM 29 O GLU 1467 -18.369 6.777 ATOM 29 O GLU 1467 -18.369 6.777 ATOM 29 O GLU 1467 -13.922 6.529 6.711 1.00 38.58 ATOM 31 CA ASP 1468 -12.839 4.592 8.791 1.00 36.09 ATOM 34 ODI ASP 1468 -11.328 4.515 8.186 1.00 25.51 ATOM 36 CA ASP 1468 ATOM 37 O ASP 1468 ATOM 38 N PRO 1469 ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 27.68 ATOM 39 CD PRO 1469 ATOM 41 CB PRO 1469 ATOM 41 CB PRO 1469 ATOM 42 CG PRO 1469 ATOM 44 CR PRO 1469 ATOM 44 O PRO 1469 -14.012 0.925 10.025 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.027.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.027.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.025 10.00 27.6		-8.222	003	10 506	1.00 42.63
ATOM 12 C LEU 1465 -13.139 12.730 8.301 1.00 39.13  ATOM 14 N PRO 1466 -13.139 12.730 8.301 1.00 40.49  ATOM 15 CD PRO 1466 -10.612 11.884 6.284 1.00 40.14  ATOM 16 CA PRO 1466 -12.754 10.821 6.284 1.00 40.14  ATOM 17 CB PRO 1466 -12.754 10.821 6.284 1.00 40.90  ATOM 18 CG PRO 1466 -12.152 10.331 4.981 1.00 40.90  ATOM 19 C PRO 1466 -12.862 9.701 7.305 1.00 40.06  ATOM 20 O PRO 1466 -11.857 9.290 7.883 1.00 40.71  ATOM 21 N GLU 1467 -14.064 9.175 7.491 1.00 38.65  ATOM 22 CA GLU 1467 -14.255 8.126 8.467 1.00 39.24  ATOM 23 CB GLU 1467 -15.314 9.365 9.353 1.00 45.06  ATOM 24 CG GLU 1467 -18.369 10.250 1.00 53.51  ATOM 26 OEI GLU 1467 -18.369 10.250 10.160 1.00 53.10  ATOM 29 O GLU 1467 -13.808 6.777 7.914 1.00 36.09  ATOM 30 N ASP 1468 -12.839 4.592 8.407 1.00 28.23  ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 28.23  ATOM 33 CG ASP 1468 -11.828 4.515 8.186 1.00 25.51  ATOM 34 OD1 ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 35 OD2 ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 27.74  ATOM 38 N PRO 1469 -14.963 3.175 8.186 1.00 27.74  ATOM 39 CD PRO 1469 -14.963 3.019 9.305 1.00 27.74  ATOM 41 CB PRO 1469 -14.963 3.019 9.305 1.00 27.56  ATOM 42 CG PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60	•	702 TEII 1465 -8.01		7 739	1.00 40.93
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ATOM 15		12 0 TEI 1465 -13.13		6 726	1.00 40.49
ATOM 15 CD PRO 1466 -10.612 11.00 40.90  ATOM 16 CA PRO 1466 -12.754 10.831 4.981 1.00 40.90  ATOM 17 CB PRO 1466 -12.152 10.331 5.202 1.00 41.39  ATOM 18 CG PRO 1466 -12.862 9.701 7.305 1.00 40.90  ATOM 19 C PRO 1466 -12.862 9.701 7.305 1.00 40.96  ATOM 20 O PRO 1466 -12.862 9.701 7.883 1.00 40.71  ATOM 21 N GLU 1467 -11.857 9.290 7.883 1.00 39.24  ATOM 22 CB GLU 1467 -15.722 8.054 8.873 1.00 45.06  ATOM 23 CB GLU 1467 -15.722 8.054 8.873 1.00 50.91  ATOM 24 CG GLU 1467 -16.314 9.365 9.353 1.00 50.91  ATOM 25 CD GLU 1467 -18.369 9.252 9.699 1.00 53.15  ATOM 26 OEI GLU 1467 -18.369 8.170 9.504 1.00 53.10  ATOM 27 OE2 GLU 1467 -13.808 6.777 7.914 1.00 36.09  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71  ATOM 31 CA ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 33 CG ASP 1468 -11.328 4.515 8.186 1.00 25.88  ATOM 34 ODI ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 35 OD2 ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 38 N PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.60  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60		13 ppo 1466 -11.79		• -	1.00 39.07
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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM		CD DDO 1466 -12.75			1.00 40.90
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ATOM 19 C PRO 1466 -12.862 9.707 7.883 1.00 40.71 ATOM 20 0 PRO 1466 -11.857 9.290 7.883 1.00 40.71 ATOM 21 N GLU 1467 -14.064 9.175 7.491 1.00 38.65 ATOM 22 CA GLU 1467 -14.255 8.126 8.467 1.00 39.24 ATOM 23 CB GLU 1467 -15.722 8.054 8.873 1.00 45.06 ATOM 24 CG GLU 1467 -16.314 9.365 9.353 1.00 50.91 ATOM 25 CD GLU 1467 -18.379 8.170 9.504 1.00 53.51 ATOM 26 OEI GLU 1467 -18.379 8.170 9.504 1.00 53.10 ATOM 27 OE2 GLU 1467 -18.369 10.250 10.160 1.00 53.10 ATOM 28 C GLU 1467 -13.808 6.777 7.914 1.00 36.09 ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71 ATOM 30 N ASP 1468 -12.839 4.592 8.407 1.00 28.23 ATOM 31 CA ASP 1468 -11.328 4.515 8.407 1.00 25.51 ATOM 32 CB ASP 1468 -11.328 4.515 ATOM 33 CG ASP 1468 -11.623 2.199 7.572 1.00 26.01 ATOM 34 ODI ASP 1468 -19.777 3.187 6.962 1.00 27.68 ATOM 35 OD2 ASP 1468 -12.570 3.405 10.493 1.00 25.83 ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83 ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88 ATOM 39 CD PRO 1469 -14.963 2.079 10.294 1.00 26.69 ATOM 41 CB PRO 1469 -14.963 2.079 10.294 1.00 26.69 ATOM 42 CG PRO 1469 -14.963 2.079 10.294 1.00 27.50 ATOM 44 CB PRO 1469 -14.963 2.079 10.294 1.00 27.60 ATOM 44 CB PRO 1469 -14.963 2.079 10.294 1.00 27.51 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.295 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.295 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469		- CC PPO 1466 -10.66			1.00 40.06
ATOM 20 O PRO 1466 -11.857 9 290 7.491 1.00 38.65 ATOM 21 N GLU 1467 -14.064 9:175 7.491 1.00 38.65 ATOM 22 CA GLU 1467 -14.255 8.126 8.467 1.00 39.24 ATOM 23 CB GLU 1467 -15.722 8.054 8.873 1.00 50.91 ATOM 24 CG GLU 1467 -16.314 9.365 9.353 1.00 50.91 ATOM 25 CD GLU 1467 -17.789 9.252 9.599 1.00 53.51 ATOM 26 OE1 GLU 1467 -18.369 10.250 10.160 1.00 53.10 ATOM 27 OE2 GLU 1467 -18.369 10.250 10.160 1.00 53.10 ATOM 29 O GLU 1467 -13.808 6.777 7.914 1.00 36.09 ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71 ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 28.23 ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51 ATOM 33 CG ASP 1468 -11.328 4.515 8.186 1.00 25.51 ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 26.00 ATOM 35 OD2 ASP 1468 -13.274 3.627 9.493 1.00 27.74 ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74 ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83 ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83 ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88 ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 25.88 ATOM 40 CA PRO 1469 -14.450 3.019 9.305 1.00 25.88 ATOM 41 CB PRO 1469 -14.963 2.079 10.294 1.00 28.81 ATOM 42 CG PRO 1469 -14.963 2.079 10.294 1.00 26.69 ATOM 43 C PRO 1469 -14.963 2.079 10.024.20 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 45 N		TB C. DPO 1466 -12.86			1.00 40.71
ATOM 21 N GLU 1467 -14.064 9.173 8.467 1.00 39.24  ATOM 22 CA GLU 1467 -15.722 8.054 8.873 1.00 45.06  ATOM 23 CB GLU 1467 -16.314 9.365 9.353 1.00 50.91  ATOM 24 CG GLU 1467 -17.789 9.252 9.699 1.00 53.51  ATOM 25 CD GLU 1467 -18.379 8.170 9.504 1.00 54.15  ATOM 26 OEI GLU 1467 -18.369 10.250 10.160 1.00 53.10  ATOM 27 OE2 GLU 1467 -18.369 10.250 10.160 1.00 36.09  ATOM 28 C GLU 1467 -13.992 6.529 6.711 1.00 36.09  ATOM 29 O GLU 1467 -13.922 6.529 8.791 1.00 30.71  ATOM 30 N ASP 1468 -12.839 4.592 8.407 1.00 28.23  ATOM 31 CA ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 32 CB ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 33 CG ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 27.74  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -14.963 2.079 10.294 1.00 28.81  ATOM 42 CG PRO 1469 -14.963 2.079 10.294 1.00 27.51  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	ATOM	19 C DPO 1466 -11.85			1.00 38.65
ATOM 22 CA GLU 1467 -14.255 8.120 8.873 1.00 45.06  ATOM 23 CB GLU 1467 -15.722 8.054 8.873 1.00 45.06  ATOM 24 CG GLU 1467 -16.314 9.365 9.353 1.00 50.91  ATOM 25 CD GLU 1467 -17.789 9.252 9.699 1.00 53.51  ATOM 26 OEI GLU 1467 -18.379 8.170 9.504 1.00 54.15  ATOM 27 OE2 GLU 1467 -18.369 10.250 10.160 1.00 53.10  ATOM 28 C GLU 1467 -13.808 6.777 7.914 1.00 36.09  ATOM 29 O GLU 1467 -13.922 6.529 8.791 1.00 30.71  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71  ATOM 31 CA ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 32 CB ASP 1468 -11.328 4.515 7.522 1.00 27.68  ATOM 33 CG ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 34 ODI ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 39 CD PRO 1469 -14.963 3.019 9.305 1.00 25.88  ATOM 40 CA PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60	MOTA	1467 -14.06			1.00 39.24
ATOM 23 CB GLU 1467	MOTA	21 N CIII 1467 -14.25			1.00 45.06
ATOM 24 CG GLU 1467 -16.314 9.305 9.699 1.00 53.51  ATOM 25 CD GLU 1467 -17.789 9.252 9.699 1.00 53.51  ATOM 26 OE1 GLU 1467 -18.369 10.250 10.160 1.00 53.10  ATOM 27 OE2 GLU 1467 -18.369 10.250 10.160 1.00 53.10  ATOM 28 C GLU 1467 -13.808 6.777 7.914 1.00 36.09  ATOM 29 O GLU 1467 -13.922 6.529 6.711 1.00 38.58  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71  ATOM 31 CA ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 33 CG ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 34 OD1 ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 27.74  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 40 CA PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 41 CB PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	22 CR CI 1467 -15.72			1.00 50.91
ATOM 25 CD GLU 1467 -17.789 9.232 9.504 1.00 54.15  ATOM 26 OEI GLU 1467 -18.379 8.170 9.504 1.00 53.10  ATOM 27 OE2 GLU 1467 -18.369 10.250 10.160 1.00 53.10  ATOM 28 C GLU 1467 -13.808 6.777 7.914 1.00 36.09  ATOM 29 O GLU 1467 -13.922 6.529 6.711 1.00 38.58  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71  ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 28.23  ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 34 ODI ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 35 OD2 ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 36 C ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	23 CT 1467 -16.3	_		1.00 53.51
ATOM 26 OE1 GLU 1467 -18.379 8.170 10.160 1.00 53.10  ATOM 27 OE2 GLU 1467 -18.369 10.250 10.160 1.00 36.09  ATOM 28 C GLU 1467 -13.808 6.777 7.914 1.00 36.09  ATOM 29 O GLU 1467 -13.922 6.529 6.711 1.00 38.58  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71  ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 28.23  ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 33 CG ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 40 CA PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.50  ATOM 43 C PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49	ATOM	CD CIT 1467 -17.7			1.00 54.15
ATOM 27 OE2 GLU 1467 -18.369 10.230 7.914 1.00 36.09  ATOM 28 C GLU 1467 -13.808 6.777 7.914 1.00 38.58  ATOM 29 O GLU 1467 -13.922 6.529 6.711 1.00 30.71  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 30.71  ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 28.23  ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 33 CG ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 27.74  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	23 CTI 1467 -18.3			1.00 53.10
ATOM 28 C GLU 1467 -13.808 6.77 6.711 1.00 38.58  ATOM 29 O GLU 1467 -13.922 6.529 6.711 1.00 30.71  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 20.71  ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 28.23  ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51  ATOM 33 CG ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	28 022 CIII 1467 -18.3			1.00 36.09
ATOM 29 O GLU 1467 -13.922 6.529 8.711 1.00 30.71  ATOM 30 N ASP 1468 -13.272 5.929 8.791 1.00 28.23  ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 25.51  ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 27.68  ATOM 33 CG ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 27.60  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 27.60	MOTA	27 OLZ -13.8	= -		1 00 38.58
ATOM 30 N ASP 1468 -13.272 5.929 8.407 1.00 28.23 ATOM 31 CA ASP 1468 -12.839 4.592 8.407 1.00 28.23 ATOM 32 CB ASP 1468 -11.328 4.515 8.186 1.00 25.51 ATOM 33 CG ASP 1468 -10.885 3.207 7.529 1.00 27.68 ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 26.01 ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 28.87 ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74 ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83 ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88 ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25 ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69 ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81 ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 27.51 ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49 ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	28 ( GH5 - 13.9	22 6.52		1.00 30.71
ATOM 31 CA ASP 1468 -12.839 4.515 8.186 1.00 25.51  ATOM 32 CB ASP 1468 -10.885 3.207 7.529 1.00 27.68  ATOM 33 CG ASP 1468 -10.885 3.207 7.529 1.00 26.01  ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 26.01  ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 28.87  ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 40 CA PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 27.60	MOTA	29 0 GEO 11-1 NCD 1468 -13.2	72 5.92	_	1 00 28.23
ATOM 31 CA ASP 1468 ATOM 32 CB ASP 1468 ATOM 33 CG ASP 1468 ATOM 34 OD1 ASP 1468 ATOM 35 OD2 ASP 1468 ATOM 36 C ASP 1468 ATOM 37 O ASP 1468 ATOM 38 N PRO 1469 ATOM 39 CD PRO 1469 ATOM 40 CA PRO 1469 ATOM 41 CB PRO 1469 ATOM 42 CG PRO 1469 ATOM 43 C PRO 1469 ATOM 43 C PRO 1469 ATOM 44 O PRO 1469 ATOM 45 N ARG 1470 ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	MOTA	30 1 1468 -12.8			1 00 25.51
ATOM 32 CB ASP 1468 -10.885 3.207 7.523 1.00 26.01  ATOM 34 OD1 ASP 1468 -11.623 2.199 7.572 1.00 28.87  ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 27.74  ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 24.20  ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 43 C PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	31 CA ASP 1468 -11.5	328 4.51	·	- 00 07 68
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ATOM 35 OD2 ASP 1468 -9.777 3.187 6.962 1.00 27.74  ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 27.74  ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.83  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -14.963 2.079 10.294 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 27.60	ATOM	33 co 146811.			07
ATOM 36 C ASP 1468 -13.274 3.627 9.493 1.00 25.83  ATOM 37 O ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 38 N PRO 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 24.20  ATOM 42 CG PRO 1469 -16.702 0.925 10.625 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	ATOM	34 ODI 1468 -9.			7 71
ATOM 36 C ASP 1468 -12.570 3.405 10.493 1.00 25.88  ATOM 37 O ASP 1469 -14.450 3.019 9.305 1.00 25.88  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 24.20  ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 43 C PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 27.60	MOTA	35 OD2 ASE 1468 -13.	274 3.62		00
ATOM 38 N PRO 1469 -14.450 3.019 9.303 1.00 24.25  ATOM 39 CD PRO 1469 -15.396 3.175 8.183 1.00 24.25  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 26.69  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 28.81  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 24.20  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 43 C PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	36 C ASE 110 -12.	570 3.40		- 00 25 98
ATOM 39 CD PRO 1469 -15.396 3.173 10.294 1.00 26.69  ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 24.20  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 27.51  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	37 U ASE 214.	450 3.03		
ATOM 40 CA PRO 1469 -14.963 2.079 10.294 1.00 28.81  ATOM 41 CB PRO 1469 -16.255 1.586 9.641 1.00 24.20  ATOM 42 CG PRO 1469 -16.702 2.776 8.816 1.00 24.20  ATOM 43 C PRO 1469 -14.012 0.925 10.625 1.00 27.51  ATOM 43 C PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60  ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49  ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	MOTA	38 N PRO 1469 -15.	396 3.1		
ATOM 40 CA PRO 1469 -16.255 1.586 9.641 1.00 24.20 ATOM 41 CB PRO 1469 -16.702 2.776 8.816 1.00 24.20 ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.51 ATOM 43 C PRO 1469 -14.012 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49 ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60	ATOM	39 CD PRO 1469 -14.	963 2.0		
ATOM 41 CB PRO 1469 -16.702 2.776 8.816 1.00 27.51 ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 43 C PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49 ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60		40. CA PRO 200 -16	255 1.5		
ATOM 42 CG PRO 1469 -14.012 0.925 10.625 1.00 27.60 ATOM 43 C PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 44 O PRO 1469 -14.172 0.285 11.657 1.00 27.60 ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 26.49 ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60		41 CB PRO 1169 -16	702 2.7	_	
ATOM 43 C PRO 12469 -14.172 0.285 11.637 1.00 26.49 ATOM 44 O PRO 1469 -13.075 0.642 9.720 1.00 26.49 ATOM 45 N ARG 1470 -13.075 0.435 9.935 1.00 27.60		42 CG PRO 1469 -14		25 10.62	
ATOM 45 N ARG 1470 -13.075 0.642 9.720 1.00 27.60 ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00 27.60		43 C PRO 2200 -14	.172 0.2		
ATOM 45 N ARG 1470 -12.108 -0.435 9.935 1.00		44 0 PRO 113	.075 0.6		27 60
CD ARG 14/0		45 N ARG -12	108 -0.4	435 9.93	35 1.00 27.80
	ATOM				



ATOM 47 CB ARG 1470 ATOM 48 CG ARG 1470 ATOM 49 CD ARG 1470 ATOM 50 NE ARG 1470 ATOM 51 CZ ARG 1470 ATOM 52 NH1 ARG 1470 ATOM 53 NH2 ARG 1470 ATOM 54 C ARG 1470 ATOM 55 O ARG 1470 ATOM 57 CA TRP 1471 ATOM 58 CB TRP 1471 ATOM 59 CG TRP 1471 ATOM 59 CG TRP 1471 ATOM 60 CD2 TRP 1471 ATOM 61 CE2 TRP 1471 ATOM 62 CE3 TRP 1471 ATOM 64 CE3 CE3 TRP 1471 ATOM 65 CE3 TRP 1471 ATOM 65 CE3 TRP 1471 ATOM 66 CE3 CE3 TRP 1471 ATOM 67 CE3 TRP 1471 ATOM 68 CE3 CE3 TRP 1471 ATOM 68 CE3 CE3 TRP 1471 ATOM 69 CE3 C
ATOM 49 CD ARG 1470 -12.073 -1.125 7.439 1.00 30.77  ATOM 50 NE ARG 1470 -11.153 -1.257 6.213 1.00 31.66  ATOM 51 CZ ARG 1470 -10.462 0.001 5.915 1.00 30.94  ATOM 52 NH1 ARG 1470 -9.577 0.167 4.941 1.00 33.30  ATOM 53 NH2 ARG 1470 -9.249 -0.846 4.144 1.00 32.78  ATOM 54 C ARG 1470 -8.990 1.346 4.779 1.00 27.16  ATOM 55 O ARG 1470 -11.116 -0.163 11.069 1.00 28.73  ATOM 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.30  ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 26.33  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.110 -0.104 11.205 1.00 23.37
ATOM 50 NE ARG 1470 -11.153 -1.257 6.213 1.00 30.77  ATOM 51 CZ ARG 1470 -10.462 0.001 5.915 1.00 30.94  ATOM 52 NH1 ARG 1470 -9.577 0.167 4.941 1.00 33.30  ATOM 53 NH2 ARG 1470 -9.249 -0.846 4.144 1.00 32.78  ATOM 54 C ARG 1470 -8.990 1.346 4.779 1.00 27.16  ATOM 55 O ARG 1470 -11.116 -0.163 11.069 1.00 28.73  ATOM 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.30  ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 26.33  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.110 -9.104 11.205 1.00 23.37
ATOM 50 NE ARG 1470 -10.462 0.001 5.915 1.00 30.77  ATOM 51 CZ ARG 1470 -9.577 0.167 4.941 1.00 30.94  ATOM 53 NH2 ARG 1470 -9.249 -0.846 4.144 1.00 32.78  ATOM 54 C ARG 1470 -8.990 1.346 4.779 1.00 27.16  ATOM 55 O ARG 1470 -11.116 -0.163 11.069 1.00 28.73  ATOM 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.30  ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 26.33  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.110 -0.104 11.205 1.00 23.37
ATOM 51 CZ ARG 1470 -9.577 0.167 4.941 1.00 30.94  ATOM 52 NH1 ARG 1470 -9.577 0.167 4.941 1.00 33.30  ATOM 53 NH2 ARG 1470 -8.990 1.346 4.144 1.00 32.78  ATOM 55 O ARG 1470 -11.116 -0.163 11.069 1.00 27.16  ATOM 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.30  ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 26.33  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 52 NH1 ARG 1470 -9.577 0.167 4.941 1.00 33.30 ATOM 53 NH2 ARG 1470 -8.990 1.346 4.144 1.00 32.78 ATOM 55 O ARG 1470 -11.116 -0.163 11.069 1.00 27.16 ATOM 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.30 ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 27.98 ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87 ATOM 60 CD2 TRP 1471 -7.110 -0.104 11.205 1.00 23.37 ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.37
ATOM 53 NH2 ARG 1470 -8.990 1.346 4.144 1.00 32.78 ATOM 55 O ARG 1470 -11.116 -0.163 11.069 1.00 27.16 ATOM 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.30 ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 27.98 ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87 ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 23.87 ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 54 C ARG 1470 -8.990 1.346 4.779 1.00 27.16  ATOM 55 O ARG 1470 -10.588 -1.091 11.069 1.00 28.73  ATOM 57 CA TRP 1471 -10.871 1.107 11.363 1.00 27.30  ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 27.98  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 24.61  ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 55 O ARG 1470 -11.116 -0.163 11.069 1.00 27.16 ATOM 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.30 ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 27.98 ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87 ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 24.61 ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 56 N TRP 1471 -10.588 -1.091 11.673 1.00 28.73  ATOM 57 CA TRP 1471 -9.892 1.107 11.363 1.00 27.30  ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 26.33  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 24.61  ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 57 CA TRP 1471 -10.871 1.107 11.363 1.00 27.30  ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 26.33  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 24.61  ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 58 CB TRP 1471 -9.892 1.430 12.375 1.00 27.98  ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 23.87  ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 24.61  ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 59 CG TRP 1471 -8.642 1.964 11.671 1.00 26.33  ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 24.61  ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 60 CD2 TRP 1471 -7.998 0.947 10.795 1.00 23.87 ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 23.33
ATOM 61 CE2 TRP 1471 -7.110 -0.104 11.205 1.00 24.61
ATOM 57 1471 -6 733 11.205 1.00 23 33
Amov 10.041 1 00 24
63 CD1 TRP 1471
3move 3446 1 00 00
65 CZ2 TRP 1471 7.369 -6.220 8.980 1.00 00
66 CZ3 TRP 1471 -1.898 10.083 1 00.02
67 CH2 TRP 1471
Alom 68 C TPD 14-2 -5.364 -2.265 11 206
69 O TDD 1472 2.384 13 470
70 N CITY 13- 3.551 2.544 14 455
ATOM 71 CA CITY -11.464 2.975 13 264 37
ATOM 72 CB CITY -11.909 3.959 3.
ATOM 73 CG CI 1 13.168 4.674 13 221
ATOM 74 CD CIU -13.497 6.026 14.402 1.00 28.25
ATOM 75 OF1 CIU 1472 -12.611 7.180 14.043 1.00 27.47
76 000 000 000 000 000 000 000 000 000 0
ATOM 77 C CIN -12.658 8.247 14 602 1.00 24.60
ATOM 78 0 -12.179 3 423 1.00 23.70
ATOM 79 N -12.795 2.735 1.00 25.89
ATOM 80 C2 -11.689 4 121 13.691 1.00 27.74
ATOM 81 CD 1473 -11.961 1.745 1.00 25.95
ATOM 82 00 1473 -10.707 3 31 18.129 1.00 27.45
ATOM 82 07 1473 -10.958 2 000 1.00 24.99
ATOM 84 -11.551 1.602 20.392 1.00 21.80
ATOM . 95 20.627 1.00 20.63
ATOM 96 1473 -12.478 5.23 21.157 1.00 22.34
ATOM 07 LEU 1473 -12 007 18.752 1.00 29 37
ATOM PRO 1474 -13 520 0.101 18.405 1.00 27 56
ATOM 1474 -14 300 19.585 1.00 30 02
ATOM 1474 -14 124 19.737 1.00 29 18
PRO 1474 15 - 20.267 1 00 20 05
91 CG PRO 1474 -15 701 5.406 21.062 1.00 26 82
ATOM 92 C PRO 1474 13.701 4.307 20.158 1.00 26.35
93 O PRO 1474 13.099 6.715 21.178 1 00 23
94 N ARG 1475 12.310 6.042 21.850 1.00 32
95 CA ARG 1475 8.038 21.178 1 00 21
96 CB ARG 1475 12.181 8.810 21.973 1 00 20
97 CG ARG 1475 10.292 21.791 1 00 25
ATOM 98 CD ARG 1475 -12.082 10.729 20.413 1 00 35.87
-11.984 12.220 1.00 43.88
SSSD/55034 VO



ATOM	99	NE	ARG	1475	-11.665	12.499	18.846	1.00	48.59
ATOM	100	CZ	ARG	1475	-10.435	12.663	18.374	1.00	46.00
ATOM	101	NH1	ARG	1475	-9.400	12.618	19.202	1.00	46.56
ATOM	102	NH2	ARG	1475	-10.241	12.746	17.065	1.00	44.18
A'TOM	103	С	ARG	1475	-12.175	8.456	23.442	1.00	35.47
ATOM	104	0	ARG	1475	-11.115	8.400	24.072	1.00	37.44
ATOM	105	N	ASP	1476	-13.347	8.134	23.974	1.00	35.04
ATOM	106	CA	ASP	1476	-13.468	7.800	25.380	1.00	34.30
ATOM	107	CB	ASP	1476	-14.940	7.853	25.797	1.00	36.89
ATOM	108	CG	ASP	1476	-15.796	6.818	25.089	1.00	38.67
ATOM	109	OD1	ASP	1476	-15.288	6.056	24.234	1.00	41.19
ATOM	110	OD2	ASP	1476	-16.995	6.758	25.406	1.00	48.08
ATOM	111	C	ASP	1476	-12.858	6.457	25.770	1.00	33.67
MOTA	112	O	ASP	1476	-12.830	6.109	26.949	1.00	36.57
ATOM	113	N	ARG	1477	-12.441	5.670	24.781	1.00	
MOTA	114	CA	ARG	1477	-11.828	4.370	25.033	1.00	29.68
ATOM	115	CB	ARG	1477	-12.117	3.418	23.886	1.00	25.53
ATOM	116	CG	ARG	1477	-13.564	3.189	23.599		23.83
ATOM	11.7	CD	ARG	1477	-14.234	2.525	24.772		26.80
MOTA	118	NE	ARG	1477	-14.493	3.485	25.842	1.00	27.24
ATOM	119	CZ	ARG	1477	-14.818	3.145	27.085	1.00	27.41
ATOM	120	NH1	ARG	1477	-14.931	1.874	27.438	1.00	29.00
ATOM	121	NH2	ARG	1477	-15.005	4.095	27.985	1.00	25.85
ATOM	122	C	ARG	1477	-10.316	4.489	25.177	1.00	30.44
ATOM	123	0	ARG	1477	<b>~9.616</b>	3.515	25.461	1.00	32.78
MOTA	124	N	LEU	1478	-9.800	5.690	25.002	1.00	30.39
ATOM	125	CA	LEU	1478	-9.370	5.883	25.080	1 00	31.96
MOTA	126	CB	LEU	1478	-7.886	6.508	23.771	1.00	30.43
ATOM	127	CG	LEU	1478	-6.400	6.424	23.431	1.00	31.90
ATOM	128	CD1	LEU	1478	-5.939	4.964	23.382	1.00	28.92
ATOM	129	CD2	LEU	1478	-6.159	7.115	22.102	1.00	33.55
ATOM	130	С	LEU	1478	-7.974	6.757	26.265	1.00	33.60
MOTA	131	0	LEU	1478	-8.193	7.972	26.251	1.00	33.96
ATOM	132	N	VAL	1479	-7.416	6.140	27.305	1.00	33.54
ATOM	133	CA	VAL	1479	-6.974	6.902	28.468	1.00	32.52
ATOM	134	CB	VAL	1479	~7.085	6.089	29.757	1.00	32.76
ATOM	135	CG1	VAL	1479	-6.728	6.973	30.926	1.00	33.27
MOTA	136	CG2	VAL	1479	-8.493	5.537	29.913	1.00	30.15
ATOM	137	C	VAL	1479	-5.529	7.341	28.239	1.00	34.24
MOTA	138	0	VAL	1479	-4.581	6.546	28.350	1.00	32.24
ATOM	139	N	LEU	1480	-5.381	8.607	27.867	1.00	35.88
ATOM	140	CA	LEU	1480	-4.077	9.192	27.569	1,00	38.43
ATOM	141	CB	LEU	1480	-4.241	10.541	26.855	1.00	36.93
ATOM	142	CG	LEU	1480	-4.828	10.535	25.435	1.00	35.67
ATOM	143		LEU	1480	-4.762	11.952	24.907	1.00	32.47
ATOM	144	CD2		1480	-4.037	9.613	24.499	1.00	33.60
ATOM	145	C	LEU	1480	-3.144	9.324	28.768	1.00	39.70
ATOM	146	0	LEU	1480	-3.511	9.912	29.784	1.00	39.88
ATOM	147	N	GLY	1481	-1.912	8.842	28.610	1.00	39.70
ATOM	148	CA	GLY	1481	-0.960	8.896	29.700	1.00	41.31
ATOM	149	С	GLY	1481	0.349	9.633	29.474	1.00	44.39
ATOM	150	0	GLY	1481	0.429	10.626	28.744	1.00	45.69

AT		l N L	YS 1482					
AT			YS 1482			.122 30	.124 1.00 44.73	,
ATO			YS 1482		728 9.		.069 1.00 46.91	,
ATO			YS 1482			934 31	.023 1.00 51.20	
ATC			'S 1482	5.1		056 30	.744 1.00 57.10	
ATO		CE L	S 1482	5.8		826 31.	248 1.00 60.81	
ATO		NZ LY		5.4		567 30.	515 1.00 61.24	
ATO		C LY		6.2		375 30.	912 1.00 65.39	
ATO:		O LY	_	3.3		782 28.	681 1.00 46.09	
ATO		N PR		3.4		782 27.	944 1.00 42.98	
ATO	~01	CD PR		3.8	-	969 28.	324 1.00 46.65	
ATON	-02	CA PR		3.9	-	L84 29.	152 1.00 46.11	
ATON		CB PR		4.53	_	212 27.6	036 1.00 45.96	
ATOM		CG PR		5.01	_	60 27.1	172 1.00 43.59	
ATOM		C PRO		4.04		53 28.1	1.00 45.37	
ATOM		O PRO		5.73		79 26.9		
ATOM		N LE		6.50		39 <sub>27.8</sub>		
ATOM		CA LEU		5.84	_	79 25.7		
ATOM		CB LEU		6.97		84 25.5		
ATOM	170	CG LEU		6.54		26 24 8		
ATOM	171	CD1 LEU		5.65		37 25.5		
ATOM	172	CD2 LEU	1484	5.063		22 24.6		
ATOM	173	C LEU	1484	5.446		0. 26.66		
ATOM	174	O LEU	1484	8.058		9 24.76		
ATOM	175	N GLY	1485	9.241		5 24.89		
ATOM	176	CA GLY	1485	7.643		6 23.93		
ATOM	177	C GLY	1485	8.603		0 23.14		
ATOM	178 (	) GLY	1485	7.997		5 22.01	6 1.00 62.66	
ATOM	179 1	V GLN	1491	6.774	12.09	21.92		
ATOM	180 (	'A GLN	1491	4.704	14.429	5 13.90		
MOTA	181 (	B GLN	1491	4.339	13.869	20.20		
ATOM	182 (		1491	3.373	14.829	20.91	8 1.00 44.31	
ATOM	183 C	GLN	1491	3.755	12.433		1.00 43.09	
ATOM	184 N	VAL	1492	2.807	12.150		1.00 43.67	
ATOM	185 C	A VAL	1492	4.338	11.542		1.00 40.40	
ATOM	-186 C	B VAL	1492	3.903	10.143		1.00 39.95	
ATOM	187 C	G1 VAL	1492	4.962	9.119		1.00 37 64	
ATOM	188 C	32 VAL	1492	4.416	7.721	20.897	1.00 34 94	
ATOM	189 C	VAL	1492	5.336 3.720	9.296	19.233	1.00 40.26	
ATOM	190 O	VAL	1492	4.679	9.905	22.586	1.00 40.23	
ATOM	191 N		1493	2.516	10.038	23.355	1.00 40.41	
ATOM	192 CA		1493	2.250	9.518	22.993	1.00 38.15	
ATOM	193 CE	VAL	1493	1.131	9.291	24.405	1.00 37.11	
ATOM		1 VAL	1493		10.245	24.924	1.00 37.83	
ATOM	195 CG		493	-0.252	11.656	24.422	1.00 36.45	
ATOM	196 C		493	1.854	9.769	24.508	1.00 39.28	
ATOM	197 0		493		7.844	24.701	1.00 36.02	
ATOM	198 N		494	1.450	7.118	23.797	1.00 37.17	
ATOM	199 CA		494	2.052 1.645	7.418	25.944	1.00 32.77	
ATOM	200 CB	<b>-</b>	494	2.445	6.081	26.335	1.00 30.87	
ATOM	201 CG		494		5.587	27.550	1.00 27.22	
ATOM	202 CD1		494	1.970	4.250	28.141	1.00 28.67	
		_	-	2.124	3.132	27.129	1.00 27.40	

ATOM	203	CD2	LEU	1494	2.736	3.904	29.377	1.00 28.84
MOTA	204	С	LEU	1494	0.173	6.256	26.701	1.00 31.18
MOTA	205	0	LEU	1494	.0.249	7.344	27.119	1.00 30.88
ATOM	206	N	ALA	1495	-0 626	5.223	26.477	1.00 30.40
ATOM	207	CA	ALA	1495	-2.044	5.307	26.817	1.00 28.30
ATOM	208	CB	ALA	1495	-2.815	5.999	25.691	1.00 27.35
ATOM	209	С	ALA	1495	-2.608	3.919	27.057	1.00 26.32
MOTA	210	0	ALA	1495	-1.926	2.915	26.846	1.00 24.54
ATOM	211	N	GLU	1496	-3.836	3.867	27.552	1.00 28.11
ATOM	212	CA	GLU	1496	-4.51.4	2.603	27.793	1.00 29.22
MOTA	21.3	CB	GLU	1496	-4.841	2.441	29.272	1.00 31.77
ATOM	214	CG	GLU	1496	-3.627	2.233	30.140	1.00 37.26
ATOM	215	CD	GLU	1496	-3.950	2.405	31.613	1.00 39.77
ATOM	216	OE1	GLU	1496	-4.322	3.534	31.999	1.00 37.54
ATOM	217	OE2	GLU	1496	-3.835	1.417	32.378	1.00 41.52
ATOM	218	С	GLU	1496	-5.799	2.594	26.970	1.00 29 76
ATOM	219	0	GLU	1496	-6.593	3.543	27.020	1.00 31.39
ATOM	220	N	ALA	1497	-5.961	1.561	26.153	1.00 29.55
ATOM	221	CA	ALA	1497	-7.139	1.426	25.324	1.00 28.69
ATOM	222	CB	ALA	1497	-6.742	0.969	23.930	1.00 23.86
ATOM	223	C	ALA	1497	8.068	J.418	25.965	1.00 29.51
ATOM	224	O	ALA	1497	-7.657	-0.762	26.278	1.00 30.40
ATOM	225	N	ILE	1498	-9.313	0.823	26.201	1.00 31.33
ATOM	226	CA	ILE	1498	-10.302	. 0.064	26.811	1.00 32.30
ATOM	227	CB	ILE	1498	-11.359	0.727	27.619	1.00 33.61
ATOM	228	CG2	ILE	1498	-12.233	-0.246	28.439	1.00 34.55
ATOM	229	CG1	ILE	1498	-10.690	1.745	28.545	1.00 31.99
ATOM	230	CD1	ILE	1498	-11.663	2.730	29.155	1.00 26.68
MOTA	231	C	ILE	1498	-11.023	-0.777	25.673	1.00 32.69
ATOM	232	O	ILE	1498	-11 644	-0.134	24.838	1.00 32.03
ATOM	233	N	GLY	1499	-10.917	-2.095	25.610	1.00 37.34
ATOM	234	CA	GLY	1499	-11.588	-2.822	24.554	1.00 44.45
ATOM	235	C	GLY	1499	-10.709	-3.193	23.372	1.00 50.75
MOTA	236	0	GLY	1499	-9.993	-4.205	23.438	1.00 53.68
ATOM	237	N	LEU	1500	-10.729	-2.370	22.321	1.00 51.14
ATOM	238	CA	LEU	1500	-9.963	-2.613	21.087	1.00 51.15
ATOM	239	CB	LEU	1500	-8.445	-2.677	21.345	1.00 50.85
ATOM	240	CG	LEU	1500	-7.516	-1.463	21.166	1.00 49.05
ATOM	241	CD1	LEU	1500	-6.082	-1.946	21.263	1.00 44.92
MOTA	242		LEU	1500	-7.703	-0.783	19.824	1.00 44.03
ATOM	243	С	LEU	1500	-10.420	-3.891	20.376	1.00 50.50
ATOM	244	0	LEU	1500	-10.544	-4.966	20.984	1.00 49.92
ATOM	245	N	PRO	1505	-13.321	-5.777	25.373	1.00 48.57
ATOM	246	CD	PRO	1505	-13.937	-7.111	25.286	1.00 50.09
ATOM	247	CA	PRO	1505	-14.289	-4.776	25.848	1.00 46.31
ATOM	248	СВ	PRO	1505	-15.630	-5.503	25.710	1.00 45.25
ATOM	249	CG	PRO	1505	-15.271	··6.918	26.025	1.00 48.85
ATOM	250	C	PRO	1505	-14.010	-4.321	27.294	1.00 43.31
ATOM	251	0	PRO	1505	-14.001	-3.122	27.571	1.00 42.84
ATOM	252	N	ASN	1506	-13.712	-5.272	28.178	1.00 40.46
ATOM	253	CA	ASN	1506	-13.430	-4.945	29.571	1.00 42.33
ATOM	254	СВ	ASN	1506	-14.302	-5.776	30.512	1.00 42.33
				~~~		3.770	J J . J L L	I. 00 II. 33



	TOM 25	5 CG AS	N 1506		_			
	rom 25	A.			-	5.436 3	0.382	1.00 42.68
	TOM 25			-0.		.269 3		1.00 47.11
	OM 25	- 40				.461 30		00 45.66
	OM 25	- 10		-11.9	_	.097 29		.00 42.89
AT	OM 260	TI		11.6 -11.0		.221 31		.00 43.23
ATO		24(1	3 1507	-9.6		.066 28	.949 1	.00 42.72
AТ	~~	74((	3 1507	-9.1		.186 29	.145 1	.00 42.24
ATO		111((	,	-9.4		384 28	.353 1	.00 50.39
ATC		14(0		-8.3		728 28	.992 1.	00 60.88
ATO		- 1400		-8.5		063 30	.038 1.	00 67.47
ATO		CZ ARG	1507	-8.01		401 30. 861 31.	574 1.	00 74.19
ATO		NH1 ARG	1507	-7.19			691 1.	00 79.97
ATO		NH2 ARG	1507		8 - 3.1.		406 1.	00 81.67
ATO		C ARG	1507	-8.98	2 -3.9		134 1.	00 82.38
ATON			1507	-9.45				00 38.15
ATOM	1 272		1508	7.92				00 36.46
ATOM	1 273	CA VAL	1508	-7.19	0 -2.3			00 35.19
ATOM	274	CG1 VAL	1508	-6.824	4 -1.2			00 33.82
ATOM		CG2 VAL	1508	-8.072	-0.7		-	0 30.19
ATOM		C VAL	1508	-5.948	-1.9			0 34.68
ATOM		O VAL	1508 1508	.5.912	-2.8	69 28.1		0 28.53
ATOM		N THR	1509	-5.392	-3 92	26 28.5		0 33.91
ATOM	- · · <del>-</del>	CA THR	1509	-5.427		27.1		0 34.02 0 31.32
ATOM		CB THR	1509	-4.206		7 26.4		31.32
ATOM ATOM		OG1 THR	1509	-4.492 -5.522	-3.01	5 25.0	31 1.00	30.88
ATOM		CG2 THR	1509	~3.255	-4.00	8 25.06	6 1.00	33.90
ATOM		THR	1509	-3.323	-3.64		1.00	24.49
ATOM	284 (		1509	-3.774	-1.30		9 1.00	28.74
ATOM	285 N 286 C		1510	-2.092	-0.21		9 1.00	27.29
ATOM			1510	-1.162	-1.43; -0.325		3 1.00	29.17
ATOM	288 C		.510	0.092	-0.595		1 1.00	30.55
ATOM	289 C	D 7110	510	-0.117	-0.460		8 1.00	27.23
ATOM	290 C	n	510	1.191	-0.614			34.33
ATOM	291 N		510	1.065	-1.603			40.49
MOTA	292 C		510 510	0.318	-1.067	32.245	-	48.28
ATOM	293 O		510 510	-0.813	-0.213	25.355		51.03
ATOM	294 N		511	.0.521	-1.218	24.700		29.64
ATOM	295 CA		511	-0.904	1.004	24.836	1.00	28.00
ATOM	296 CB		11	-0.625	1.305	23.446	1.00	30.10
ATOM	297 CG	• •••	11	-1.951	1.464	22.636	1.00 3	27.20
ATOM	298 CG	<b>~</b>	11	-2.719	0.143	22.615	1.00 3	10 42
ATOM	299 C	VAL 15		-2.829	2.629	23.223	1.00 2	8 00
ATOM ATOM	300 O	VAL 15		.0.150 0.274	2.626	23.365	1.00 3	0.51
	301 N	ALA 15			3.346	24.360	1.00 3	1.09
ATOM ATOM	302 CA	ALA 15			2.935	22.185	1.00 2	8.30
ATOM	303 CB	ALA 15:		_	4.173	21.979	1.00 2	5.23
ATOM	304 C	ALA 151			3.889	21.331	1.00 23	3.82
ATOM	305 O	ALA 151	.2		5.012	21.057	1.00 25	5.50
	306 N	VAL 151	3	_	4.515 6.281	20.061	1.00 27	7.06
				- (	501	21.404	1.00 29	.37

A'	rom	307	CA	VAL	1513	-0.477	7.199	20.625		31.53
	rom	308	CB	VAL	1513	-1.588	7.843	21.504		32.26
A'	rom	309	CG1		1513	-2.453	8.775	20.684	1.00	34.37
	TOM	310	CG2		1513	-2.452	6.776	22.152		33.42
	rom	311	C	VAL	1513	0.347	8.328	20.006		33.34
A.	rom	312	0	VAL	1513	1.030	9.064	20.719		32.35
A.	rom	313	N	LYS	1514	0.321	8.423	18.680	1.00	36.65
A:	rom	314	CA	LYS	1514	1.022	9.466	17.929	1.00	37.26
	MOT	315	CB	LYS	1514	1.541	8.917	16.606	1.00	36.21
A:	rom	316	CG	LYS	1514	2.524	7.792	16.800	1.00	39.32
A.	rom	317	CD	LYS	1514	2.725	6.998	15.535	1.00	42.59
A?	MOT	318	CE	LYS	1514	3.245	7.860	14.416	1.00	44.71
A?	MOT	319	NZ	LYS	1514	4.408	8.680	14.844	1.00	38.78
A'	MOT	320	С	LYS	1514	0.020	10.574	17.653	1.00	37.21
A'	MOT	321	0	LYS	1514	-1.095	10.305	17.192	1.00	37.39
ΑT	MOT	322	N	MET	1515	0.433	11.812	17.908	1.00	39.05
A'	MOT	323	CA	MET	1515	-0.419	12.981	17.713	1.00	41.68
ΑT	MOT	324	CB	MET	1515	-1.162	13.299	18.991	1.00	41.07
A1	MOT	325	CG	MET	1515	-0.251	13.641	20.139	1.00	40.69
ΑΊ	MOT	326	SD	MET	1515	-1.271	13.763	21.571	1.00	41.18
ΑΊ	MOT	327	CE	MET	1515	-1.523	12.018	21.959	1.90	40.98
ΑŢ	MOT	328	C	MET	1515	0.397	14.197	17.321	1.00	44.66
ΑΊ	MOT	329	0	MET	1515	1.606	14.255	17.550	1.00	43.83
Al	MOT	330	N	LEU	1516	-0.288	15.182	16.747	1.00	50.63
ΑT	MOT	331	CA	LEU	1516	0.349	16.423	16.312	1.00	52.21
ΑΊ	MOT	332	CB	LEU	1516	-0.513	17.129	15.255	1.00	50.18
ΓA	MO	333	CG	LEU	1516	-0.757	16.463	13.904	1.00	50.25
ΑT	MO	334	CD1	LEU	1516	-1.733	17.298	13.114	1.60	51.02
ΑT	MO	335	CD2	LEU	1516	0.555	16.329	13.163	1.00	51.60
Αī	MO	336	C	LEU	1516	0.549	17.391	17.473	100	54.25
ΑŢ	MO	337	0	LEU	1516	-0.143	17.326	19.488	1.00	52.52
ΑT	MO	338	N	LYS	1517	1.500	18.299	17.302	1.00	59.09
ΓA	MO	339	CA	LYS	1517	1.773	19.315	18.313	1.00	62.57
ΑT	MO	340	CB	LYS	1517	3.220	19.813	18.222	1.00	66.29
ΑT	MO	341	CG	LYS	1517	4.281	18.810	18.663	1.00	70.96
AT	MO	342	CD	LYS	1517	5.666	19.197	18.130	1.00	74.61
ΑT	MO	343	CE	LYS	1517	6.711	18.118	18.414	1.00	78.21
ΙA	MO	344	NZ	LYS	1517	8.020	18.410	17.751	1.00	77.95
ΑŢ	MO	345	C	LYS	1517	0.824	20.474	18.037	1.00	63.07
ΑŢ	MO	346	0	LYS	1517	0.226	20.557	16.960	1.00	63.68
ΑŢ	MO	347	N	SER	1518	0.720	21.391	18.987	1.00	64.54
ΑŢ	MO	348	CA	SER	1518	-0.167	22.543	18.848	1.00	67.29
AT	MO	349	CB	SER	1518	-0.085	23.439	20.090	1.00	65.14
ΓA	MO	350	C	SER	1518	0.124	23.382	17.609	1.00	69.48
ΑT	MO	351	0	SER	1518	-0.798	23.843	16.938	1.00	71.85
ΑT	MO	352	N	ASP	1519	1.402	23.530	17.280		70.88
ΑT	MO	353	CA	ASP	1519	1.802	24.326	16.127		72.00
ΓA	MO	354	CB	ASP	1519	3.162	24.973	16.385		72.61
ΑT	MO	355	С	ASP	1519	1.861	23.548	14.817		72.32
ΑT	MO	356	0	ASP	1519	2.432	24.035	13.844		73.72
ΑT	MO	357	N	ALA	1520	1.322	22.332	14.798		72.11
AT	MO	358	CA	ALA	1520	1.344	21.508	13.595		71.13

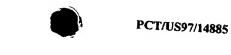


ā mos		
ATON	. OB ALA 1520	0.650
ATOM	360 C ALA 1530	0.659 20.173 13.855 1.00 71.01
ATOM	361 O ALA 1530	12.242 12.440 1 00 60 06
ATOM	362 N THR 1531	-0.314 22.962 12.639 1 00 71 41
ATOM	363 CA THR 1531	1.230 22.101 11.249 1 00 67 30
ATOM	364 CB THR 1521	0.6/6 22.726 10.064 1 00 55
ATOM	365 OG1 THR 1521	1.798 23.167 9.132 1.00
ATOM	366 CG2 THR 1521	2.521 22.016 8.680 1.00 70 75
ATOM	367 C	2.741 24.070 9 867 7 7
ATOM	368 A	-0.150 21.665 9 364 1 22
ATOM	369 N	-0.093 20.493 9 740 1 65.62
ATOM	370 Ch 222	-0.893 22.057 8 330 1 00 5
ATOM	371 CD 222	-1.698 21.095 7 584 3 00 53.60
ATOM	372 C 220	-2.560 21.802 6.531 1.00 62.25
ATOM	373 0 7522	-0.768 20 05
ATOM	374 N 377	-1.161 18 006 -1.00 60.41
ATOM	377 213 1523	0.475 20 445
ATOM	376 On	1.449 19 50.47
ATOM	377 00	2.739 20 273
ATOM	378 CD ****	3.897 19 301
ATOM	379 CD 1523	3.482 70.454
ATOM	300 35	4.681 17.222
ATOM	381 0	4.252 16 704 2 455 1.00 68.18
ATOM	302 - 215 1523	1.728 10 474 2.458 1.00 73.23
ATOM	383 17	1.757 17 200
ATOM	384 07 2524	1.899 18 037
ATOM	205 1524	2.147 18 222 8.376 1.00 47.78
ATOM	396 55	2.380 10.015
ATOM	307 - ASE 1524	3.744 19 513
ATOM	-52 ASE 1524	3.849 30.500
ATOM	300	4.715 18 004 1.00 47.22
ATOM	300 - 401 1524	0.968 17.05
ATOM	301 H	1.157 15 000 1.00 43.55
ATOM	300 1525	-0.240 17 541
ATOM	302	-1.438 16.773
ATOM	304 00	-2.701 17.500
7 CON	305 55	-4.100 16 052 J.411 1.00 40.54
) TOO	395 CD1 LEU 1525	-4.289 15 022 1.00 40.33
3.000	396 CD2 LEU 1525	-5.120 19 044
3	397 C LEU 1525	-1 417 15 600 36.98
3.000	398 O LEU 1525	-1.682 14 50F
	399 N SER 1526	-1 064 16 15
3.500.	400 CA SER 1526	-1.002 15 335 7.147 1.00 42.13
	101 CB SER 1526	-0.582 16.336 5.954 1.00 44.75
3.000.	102 OG SER 1526	1 570 - 4.723 1.00 49.61
<b>-</b>	103 C SER 1526	-0.003 17.100 4.352 1.00 59.95
T TOOL	04 O SER 1526	0 207 4 6.144 1.00 42.71
	05 N ASP 1527	3 167 5.840 1.00 45.33
3.000.	<sup>06</sup> CA ASP 1527	2 310 17 6.655 1.00 40.97
T COLO	<sup>07</sup> CB ASP 1527	3 407 6.867 1.00 41.03
70000	08 CG ASP 1527	4 000 45 30
Ti COLORA	09 OD1 ASP 1527	3 700 13.14/ 6.235 1.00 47 84
ATOM 4	10 OD2 ASP 1527	100 48.84
		4.957 15.966 6.600 1.00 49.11
SSCD/FFOR		



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ATOM	411	C	ASP	1527	1.782	12.485	7.858	1.00 39.01
ATOM	412	0	ASP	1527	2.021	11.298	7.651	1.00 40.04
MOTA	413	N	LEU	1528	1.094	12.917	8.909	1.00 35.93
ATOM	414	CA	LEU	1528	0.594	12.004	9.927	1.00 36.48
ATOM	415	CB	LEU	1528	-0.008	12.784	11.107	1.00 36.51
ATOM	416	CG	LEU	1528	-0.436	11.961	12.326	1.00 40.56
MOTA	417	CD1	LEU	1528	0.650	10.955	12.692	1.00 42.00
ATOM	418	CD2	LEU	1528	-0.770	12.877	13.499	1.00 38.25
ATOM	419	C	LEU	1528	-0.453	11.065	9.309	1.00 35.25
ATOM	420	0	LEU	1528	-0.442	9.855	9.566	1.00 36.37
MOTA	421	N	ILE	1529	-1.311	11.614	8.453	1.00 33.10
ATOM	422	CA	ILE	1529	-2.365	10.839	7.805	1.00 32.32
ATOM	423	CB	ILE	1529	-3.364	11.732	7.012	1.00 31.17
ATOM	424	CG2	ILE	1529	-4.311	10:861	6.187	1.00 32.01
ATOM	425	CG1	ILE	1529	-4.193	12.579	7.983	1.00 31.35
ATOM	426	CD1	ILE	1529	-5.024	13.662	7.335	1.00 32.59
ATOM	427	C	ILE	1529	-1.732	9.825	6.877	1.00 33.44
ATOM	428	0	ILE	1529	-2.148	8:667	ó.860	1.00 35.41
ATOM	429	N	SER	1530	-0.733	10.269	6.108	1.00 33.40
ATOM	430	CA	SER	1530	0.007	9.414	5.171	1.00 34.34
ATOM	431	CB	SER	1530	1.126	10.197	4.495	1.00 38.37
MOTA	432	ΟG	SER	1530	0.605	11.332	3.835	1.00 46.02
MOTA	433	C	SER	1530	0.614	8.208	5.968	1.00 30.41
MOTA	434	0	SER	1530	0.494	7.083	5.376	1.00 30.50
ATOM	435	N	GLU	1531	1.256	8.449	7.010	1.00 27.40
ATOM	436	CA	GLU	1531	1.865	7.369	7.766	1.00 28.90
MOTA	437	CB	GLU	1531	2.629	7.907	8.973	1.00 28.45
MOTA	438	CG	GLU	1531	3.263	6.812	9.825	1.00 29.33
ATOM	439	CD	GLU	1531	4.094	7.344	10.979	1.00 31.14
ATOM	440	OE1	GLU	1531	4.913	6.561	11.495	1.00 33.14
ATOM	441	OE2	GLU	1531	3.940	8.522	11.378	1.00 31.11
MOTA	442	C	GLU	1531	0.824	6.351	8.215	1.00 30.88
ATOM	443	0	GLU	1531	1.118	5.146	8.259	1.00 32.35
ATOM	444	N	MET	1532	-0.377	6.832	8.553	1.00 29.86
ATOM	445	CA	MET	1532	-1.476	5.966	8.996	1.00 30.01
ATOM	446	CB	MET	1532	-2.608	6.800	9.596	1.00 29.58
ATOM	447	CG	MET	1532	-3.761	5.968	10.146	1.00 31.20
MOTA	448	SD	MET	1532	-5.095	6.973	10.779	1.00 29.37
ATOM	449	CE	MET	1532	-5.271	8.228	9.489	1.00 21.59
ATOM	450	С	MET	1532	-2.002	5.145	7.814	1.00 29.60
ATOM	451	0	MET	1532	-2.131	3.923	7.893	1.00 29.68
ATOM	452	N	GLU	1533	-2.257	5.824	6.702	1.00 30.38
ATOM	453	CA	GLU	1533	-2.755	5.176	5.495	1.00 30.12
ATOM	454	CB	GLU	1533	-2.987	6.221	4.423	1.00 25.79
ATOM	455	CG	GLU	1533	-4.117	7.154	4.784	1.00 26.67
ATOM	456	CD	GLU	1533	-5.420	6.405	5.064	1.00 29.90
MOTA	457	OE1	GLU	1533	-5.923	5.696	4.166	1.00 29.93
ATOM	458	OE2	GLU	1533	-5.939	6.518	6.197	1.00 29.10
MOTA	459	C	GLU	1533	-1.787	4.120	5.003	1.00 30.32
MOTA	460	0	GLU	1533	-2.197	3.043	4.563	1.00 32.06
MOTA	461	N	MET	1534	-0.500	4.435	5.136	1.00 29.97
ATOM	462	CA	MET	1534	0.606	3.571	4.737	1.00 31.22



	TOM	46	3 CB	MET	1534	
	MOT	46		MET	1534	4.305 4 995
AT	MOT	46		MET		3.118 3.487 4.675
	MO	466		MET	1534	3.528 3.627 2 982 7 00 40.40
AT	'OM	467		MET	1534	5.215 4.257 3 155 1 27
AT		468		MET	1534	0.565 2 304 - 1.00 42.49
AT		469		MET	1534	0.596
ATO		470		MET	1535	0.493
ATO		471	CB	MET	1535	0.417
ATC	MC	472	CG		1535	0.325 1 930 1.00 28.82
ATC	M	473	SD	MET	1535	1.622 2.424 1.00 28.87
ATO	M	474	CE	MET	1535	1.674 2.622
ATO	M	475	C	MET	1535	1.393 4 225 1.00 30.96
ATO	M	476	_	MET	1535	-0.777 0.460 11.729 1.00 27.69
ATO		477			1535	-0.682 -0.734 - 1.00 28.59
IOTA		478	·		1536	-1.885 1.072 7.530 1.00 30.37
ATON		479			1536	-3.078 0.315 7.019 1.00 26.53
ATON		¥80			1536	-4.237 3.353 5.608 1.00 27.60
ATOM		181			1536	14 807 5.283 1.00 25 80
ATOM					L536	-5 025
ATOM		82			153 <i>6</i>	7.061 1.00 21.64
ATOM	,	83			.536	7 460 4 8,225 1.00 21 83
ATOM	-	84	_		536	7.796 1.00 26 27
MOTA	-	85	_		536	-3 150 5.397 1.00 27 49
ATOM	_				537	-2 196 5 393 1.00 29 24
A.TOM				ET 1	537	1.372 1.00 27 80
ATOM				ET 19	537	*1 221 ** 763 3.172 1.00 29 17
ATOM			CG MI	ET 15	537	2 202 4 2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
ATOM	49		SD ME	ET 15	537	1.566 1 (0.37 1)
ATOM	4.9		E ME	T 15	37	2 004 2 0.744 1 00 43 17
ATOM	49	_ "		T 15	37	-0.9030.698 1.00 43.04
ATOM	49			T 15	37	3.447 1.00 29 58
ATOM	49			E 15	38	0.142 2.996 1.00 27 53
ATOM	49	_	A IL	E 15	38	1 100 28 64
ATOM	49	_			38	2 381 2 4,533 1.00 26,88
ATOM	49	/ C	G2 ILI	E 153	38	3 300 25 23
ATOM	498		31 ITE		38	3 007 0 5.745 1.00 27.31
ATOM	. 499		)1 ILE	153	8 8	0.300 4.345 1 00 00 m
ATOM	500	_	ILE	153	8	0.756 4.874 1.00 23 44
ATOM	501	-	ILE		8	1 274 5.224 1.00 26.75
ATOM	502	•	GLY	153	9	*0 200 2 4.909 1.00 28.60
ATOM	503	CA		153		0.625 6.137 1.00 27 19
ATOM	504	С	GLY	153	9	0.207 5.009 6.812 1.00 26 88
ATOM	505	0	GLY	153		1 220 8.039 1.00 26 04
ATOM	506	N	LYS	154(	)	-0 105 8.281 1.00 27 96
ATOM	507	CA	LYS	1540	)	8.788 1.00 23 25
ATOM	508	CB	LYS	1540		0.701 10.052 1.00 21 52
ATOM	509	CG	LYS	1540		1.500 -7.350 11.028 1.00 20 40
	510	CD	LYS	1540		2.540 -6.346 11.563 1.00 28 43
ATOM	511	CE	LYS	1540		2.542 -6.977 12.502 1.00 36 24
ATOM	512	NZ	LYS	1540		3.568 -5.942 12.994 1.00 41 05
ATOM	513	C	LYS	1540		-2.9/3 -4.847 13.836 1 00 th
ATOM	514	0	LYS	1540		1.577 -7.796 9.974 1.00 19 96
						1.536 -8.723 9.176 1.00 19.96 1.00 21.51
SSSD/FFA						ar'aT



		7 670 10.905 1.00 19.82
	3543	2.514 -7.870 200 21.35
MOTA	515 N HIS 1541	3.622 -8.613 11.040 1.00 21 39
	516 CA HIS 1541	4.704 -8.411 9.972 1.00 17 07
MOTA	51/ CB	5.747 -9.490 9.963 1.00
MOTA	518 CG HIS 1541	5.810 -10.667 9.292 1.00 19.05
ATOM	519 CD2 HIS 1541	6.891 -9.428 10.727 1.00 19 63
MOTA	520 ND1 HIS 1541	7.609 -10.522 10.535 1.00 18 32
MOTA	521 CE1 HIS 1541	c 975 -11.293 9.668 1.00 -
MOTA	522 NE2 HIS 1541	4 108 -8.456 12.449 1.00 25
MOTA	523 C HIS 1541	4.231 -7.352 13.002 1.00 24.32
MOTA	524 O HIS 1541	4.587 -9.577 13.045 1.00 -
MOTA	525 N LYS 1542	5.141 -9.610 14.396 1.00 30 70
ATOM	526 CA LYS 1542	5.578 -11.044 14.742 1.00 30.75
MOTA	527 CB LYS 1542	6.130 -11.239 16.130 1.00 48 24
MOTA	528 CG LYS 1542	6.380 -12.719 16.420 1.00 56 89
MOTA	529 CD LYS 1542	6 995 -13.414 15.183 1.00
MOTA	530 CE LYS 1542	7.457 -14.831 15.421 1.00 24 59
ATOM	531 NZ LYS 1542	C 318 8.674 14.608 1.00
MOTA	532 C LYS 1542	6 462 -8.067 15.676 1.00 23.23
MOTA	533 O LYS 1542	7.147 -8.546 13.576 1.60 21 40
ATOM	534 N ASN 1543	9 373 -7.702 13.669 3.669
MOTA	535 CA ASN 1543 536 CB ASN 1543	9.558 -8.482 13.217 1.00 20 37
MOTA	550 02	9.721 -9.811 13.945 1.00 24 97
ATOM	537	9.501 -10.883 13.372 1.00 21.56
MOTA	538 ODI AUT	10.016 -9.741 15.230 1.00 20 38
MOTA	535 102 104	8.312 -6.268 13.155 2.00 20 03
MOTA	540 C 1221	9.353 -5.733 12.776 1.00 30 02
MOTA	541 0 27 7 3544	7.153 -5.624 13.180 1.00 21 14
MOTA	542 N TIE 1544	7.037 -4.220 22 20 22 97
MOTA	543 CA == 1544	5.5454.029 22.27
MOTA	544 CD 1544	7.436 -4.810 22.85
MOTA	545 CG2 22-	5.082 -4.447 22.00 1 00 18.94
MOTA	546 CGI 122	4.485 -3.974 1.00 20.02
MOTA	34, 65- 15/4	6.044 -3.590 14 466 1 00 21.00
MOTA	540 C 1544	5.342 -4.303 221 1 00 20.09
MOTA	545 C 1545	6.103 2.273 2.4 926 1.00 22.82
MOTA	TTE 1545	5.140 -1.808 27.109 1.00 23.07
MOTA	551 CR TLE 1545	5.586 -0.101 25 718 1.00 21.94
MOTA	552 CG2 TLE 1545	4.399 0.652 16 193 1.00 20.49
MOTA	554 CC1 TLE 1545	6.759 -0.178 131-1
ATOM	1 554 555 TER 1545	6.450 -0.730 1.00 1.00 24.18
MOTA	TLE 1545	3.853 -1.333 -20 1 00 25.68
MOTA	M 556 C 1545	3.809 -0.934
OTA	M 557 0 25N 1546	2.829 -2.230 231 13.853 1.00 24.23
OTA	M 558 Ch ASN 1546	1.528 -2.311 13.060 1.00 25.21
OTA	M 559 CR ASN 1546	0.866 -3.837 13 481 1.00 21.10
ATO	M 560 CC ASN 1546	1.690 -4.651 -1.00 23.44
OTA	M 561 CO 1546	1.764 -4.997 14.343 1.00 18.20
ATO	M 502 DD2 ASN 1546	2.324 -3.606 221 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
OTA	OM 563 REZ ASN 1546	0.567 -1.233 15 426 1.00 24.14
OTA	OM 564 C ASN 1546	0.709 -0.882 23.49
TA	OM 565 0 LEI 1547	-0.382 -0.920 13.456 1.00 23.13
ATO	OM 566 N LEU 134,	

А	TOM 567 CA TOW	
	MOSS CW LEO	1547
	MOTE TEO	1547 0.069 13.718 1.00 24 24
	TEO TEO	1547 0.597 12.378 1 00 21 52
	TOM 570 CD1 LEU	1547
	10M 571 CD2 1777	2.834 2.903 12 922
	10M 572 C 7 TTT	1.660 10 020
	TOM 573 O True	2.510 -0.681 14 405
	OM 574 N LEU	-2.849 -1.823 14 160 26.70
	OM 575 CA 1511	-3.017 -0.082 15 505 -1.00 28.96
AT	OM 576 CB LETT	-4.047 -0.714 16 365 a
AT	OM 577 CG 1877	-3.686 -0.682 17.860
ATO	OM 578 CD1 1.Ftt 7	-2.346 -1.360 18 224
ATC	$^{\text{JM}}$ 579 CD2 $^{\text{TD2}}$	-2.150 -1 460 -1 1.00 17.12
ATC	OM 580 C 180	.548 -2.266 -2.737 13.708 1.00 18.81
ATO	M Ees D	-5.395 -0.061 17.631 1.00 16.20
ATO	M 582 N 555	548 -6.418 -0.737 16.099 1.00 23.30
ATO	M 502 CT GDI 1	549 -5.395 1 320 10.175 1.00 24.18
ATO	M 504 C GLI I	-6.636 1 932 -5.758 1.00 21.53
ATO	M 505 0 GLY 15	-6.392 3 403 15.485 1.00 22.47
ATOM	M SOC 15	13.340 1.00 24 62
ATOM	1 503 - ALA 15	250 -7 450 131.63 1.00 25 06
ATOM	1 ESS CA ALA 15	50 -7 362 5 555 13.409 1.00 24.15
ATOM	CB ALA 15	50 "7 053 5 13.313 1.00 22 20
ATOM	ALA 15	50 -8 500 13.890 1.00 19 97
ATOM	501 15 ALA 1.5	50 -9 707 " 07 15,802 1,00 23,75
ATOM	500 CTS 15	51 -8 383 -15.804 1.00 26 43
ATOM	501 CA CYS 155	51 -9 425 0 50 10 25 34
ATOM	504 55	10.6/8 1.00 27 17
ATOM	- 610 100	18.127 1.00 26 84
ATOM	595 C CYS 155	1 -9 204 1.00 30 32
ATOM	596 O CYS 155	1 -8 364 -1 15./19 1.00 28 42
ATOM	597 N THR 155	210 145 15.827 1.00 27 28
ATOM	598 CA THR 155	2 -10 076 10 14.702 1.00 30 47
ATOM	599 CB THR 155	2 10.078 10.873 13.690 1 00 22
ATOM	600 OG1 THR 1552	2 4 44.280 1 00 20
ATOM	601 CG2 THR 1552	2 -9 905 12.096 1.00 31 11
ATOM	602 C THR 1552	9.255 12.151 1 00 27
ATOM	603 O THR 1552	
ATOM	604 N GLN 1553	12.911 13.070 1 00 20 7
ATOM	605 CA GLN 1553	12.339 11.408 14.286 1 00 35
ATOM	606 CB GLN 1553	- 14.295 1 00 30
ATOM	607 CG GLN 1553	14.775 11.359 14.148 1 00 7
ATOM	608 CD GLN 1553	10.529 12.876 7.00
ATOM	609 OE1 GLN 1553	11.381 11.627 1.00
	610 NE2 GLN 1553	13.442 12.345 11.445 1 00 45
ATOM	bll C GLN 1553	13.746 11.033 10.765 1 00 10
ATOM	612 O GLN 1553	13.038 13.168 15.483 1 00 13.32
ATOM	613 N ASP 1554	-13.230 12.837 16.590 1.00 20 20
ATOM	614 CA ASP 1554	-14.225 14.344 15.219 1 00 44 F
ATOM	615 CB ASP 1554	-14.474 15.356 16 227
ATOM	616 CG ASP 1554	-15.778 15.028 15 025 1.00 46.94
ATOM	617 OD1 ASP 1554	-17.007 15.262 16 100 49.94
ATOM	610 0-	-17.966 15.878 16 635 1.00 56.68
	OD2 ASP 1554	-17.030 14 020 4.00 64.76
COOP		14.829 14.947 1.00 60.79

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ATOM	619	C	ASP	1554	-13.343	15.563	17.244	1.00 47.24
MOTA	620	0	ASP	1554	-13.522	15.375	18.452	1.00 48.98
MOTA	621	N	GLY	1555	-12.182	15.966	16.747	1.00 44.00
ATOM	622	CA	GLY	1555	-11.062	16.185	17.638	1.00 41.07
MOTA	623	C	GLY	1555	-9.728	15.891	16.994	1.00 40.26
ATOM	624	0	GLY	1555	-9.663	15.567	15.810	1.00 39.72
MOTA	625	N	PRO	1556	-8.635	15.987	17.759	1.00 39.21
ATOM	626	CD	PRO	1556	-8.634	16.266	19.208	1.00 39.09
ATOM	627	CA	PRO	1556	-7.271	15.740	17.294	1.00 37.84
MOTA	628	CB	PRO	1556	-6.436	15.947	18.549	1.00 39.66
ATOM	629	CG	PRO	1556	-7.269	16.842	19.389	1.00 39.53
ATOM	630	C	PRO	1556	-7.094	1.4.314	16.806	1.00 37.75
ATOM	631	0	PRO	1556	-7.574	13.377	17.444	1.00 37.25
ATOM	632	N	LEU	1557	-6.379	14.153	15.699	1.00 36.09
ATOM	633	CA	LEU	1557	-6.112	12.844	15.124	1.00 34.69
ATOM	634	CB	LEU	1557	-5.458	13.010	13.741	1.00 32.25
ATOM	635	CG	LEU	1557	-4.962	11.774	12.972	1.00 31.23
ATOM	636	CD1	LEU	1557	-6.080	10.763	12.715	1.00 25.69
ATOM	637	CD2	LEU	1557	-4.339	12.219	11.669	1.00 28.21
ATOM	638	C	LEU	1557	-5.190	12.057	16.060	1.00 34.59
ATOM	639	O	LEU	1557	-4.173	12.578	16.524	1.00 32.09
ATOM	640	Ŋ	TYR	1558	-5,606	10.841	16.396	1.00 32.63
MOTA	641	C.A	TYR	1558	-4.796	9.993	17.237	1.00 29.66
MOTA	642	CB	TYR	1558	-5.529	9.630	18.534	1.00 33.14
ATOM	643	CG	TYR	1.558	-5.588	10.754	19.539	1.00 32.87
ATOM	644	CD1	TYR	1558	-6.583	10.793	20.517	1.00 34.58
ATOM	645	CE1	TYR	1558	-6.678	11.957	21.407	1.00 34.65
ATOM-	646	CD2	TYR	1558	-4.678	11.805	19.483	1.00 35.69
ATOM	647	CE2	TYR	1558	-4.760	12.878	20.367	1.00 37.01
MOTA	648	CZ	TYR	1558	.5.766	12.899	21.324	1.00 37.52
MOTA	649	OH	TYR	1558	-5.868	13.986	22.164	1.00 40.19
MOTA	650	C	TYR	1558	-4.529	8.747	16.436	1.00 28.08
MOTA	651	0	TYR	1558	-5.467	8.137	15.924	1.00 30.12
ATOM	652	N	VAL	1559	-3.254	8.444	16.225	1.00 25 89
MOTA	653	CA	VAL	1559	-2.855	7.246	15.504	1.00 23.70
ATOM	654	CB	VAL	1559	-1.729	7.528	14.485	1.00 23.78
ATOM	655	CG1	VAL	1559	-1.456	6.282	13.623	1.00 20.75
ATOM	656	CG2	VAL	1559	-2.101	8.738	13.604	1.00 22.54
ATOM	657	С	VAL	1559	-2.358	6.311	16.596	1.00 23.47
ATOM	658	0	VAL	1559	-1.328	6.572	17.220	1.00 26.84
ATOM	659	N	ILE	1560	-3.146	5.283	16.889	1.00 23.58
ATOM	660	CA	ILE	1560	-2.818	4.316	17.928	1.00 23.75
ATOM	661	СВ	ILE	1560	-4.112	3.732	18.552	1.00 22.67
MOTA	662		ILE	1560	-3.777	2.898	19.788	1.00 20.24
ATOM	663		ILE	1560	-5.063	4.884	18.904	1.00 20.09
ATOM	664		ILE	1560	-6.428	4.463	19.318	1.00 19.04
ATOM	665	C	ILE	1560	-1.954	3.181	17.356	1.00 13.04
ATOM	666	ō	ILE	1560	-2.411	2.392	16.505	1.00 27.39
ATOM	667	N	VAL	1561	-0.720	3.089	17.840	1.00 26.76
ATOM	668	CA	VAL	1561	0.238	2.088	17.368	1.00 25.76
ATOM	669	CB	VAL	1561	1.445	2.801	16.653	1.00 23.91
ATOM	670	CG1		1561	0.952	3.480		
	3.0		A 1277	1001	0.352	3.400	15.397	1.00 13.55

) Trans		
ATOM	671 CG2 VAL 1561	
ATOM	672 C VAL 1561	4.054 3 070
ATOM	6/3 O VAL 1561	0.693 1.151 18 510
ATOM	6/4 N GLU 1563	0.39/ 1.417 19 696
ATOM	675 CA GLU 1562	0.032 18 192
ATOM	676 CB GLU 1562	1.793 -0.901 19 220
ATOM	677 CG GLU 1562	4,369 -2,179 10 636
ATOM	678 CD GLU 1563	1.312 -3.115 18 093
ATOM	679 OE1 GLU 1562	1.895 -4.356 17 460
ATOM	680 OE2 GLU 1562	1.201 -5.432 17 573
ATOM	681 C GLU 1562	2,3564.260 16 925
ATOM	682 O GLU 1562	2.802 -0.261 20.158 1 00 22 -
ATOM	683 N TYR 1563	0.578 19.738 1 00 23.36
ATOM	684 CA TYR 1563	2.787 -0.665 21.422 1 00 25
ATOM	685 CB TYR 1563	3.6// -0 132 22 442
ATOM	686 CG TYR 1563	2.907 0.035 23.744 1.00 28.98
ATOM	687 CD1 TYR 1563	3.744 0.456 24.929 1 CO 32 05
ATOM	OBS CEI TYR 1563	1.653 24.915 1 00 35.66
ATOM ATOM	689 CD2 TYR 1563	3.195 2.069 26.021 1 00 25
ATOM	090 CE2 TYR 1563	3.787 -0.322 26.082 1 00 34 85
ATOM	691 CZ TYR 1563	0.080 27.186 1 00 24 45
ATOM	692 OH TYR 1563	5.219 1.273 27.150 1 00 17 02
	693 C TYR 1563	1.662 28,228 1 00 1
	694 O TYR 1563	1.043 22.668 1 00 1
3	695 N ALA 1564	2.745 -2.269 22.751 1 00 33
A moss	696 CA ALA 1564	7 202 22.//9 1.00 31 00
7 moss	697 CB ALA 1564	3 226 22.998 1.00 11 00
<b>-</b> ·	598 C ALA 1564	7 940 21.792 1.00 30 92
Amore	10C N	8 703 0 24 283 1.00 29 32
7 Mose	101 Co	7.603 -1.303 -24.274 1.00 32.26
7 TION	02 CD 0==	8.059 -0.884 25.389 1.00 29.55
ATOM 7	03 OG SER 1565	7.392 -1 720 1.00 30.89
ATOM 7	04 C SER 1565	7.704 -3.094 27.792 1.00 29.79
	05 0 2=	9.547 -0.840 36 006
ATOM 70	76 N	9.978 -0 150 27 000 1.00 31.39
ATOM 70	O7 CA LYS 1566	10.340 -1.576 26 220 1.00 35.74
ATOM 70		11.756 -1.560 26 405
ATOM 70		12.322 -2.973 26 447
ATOM 71	O CD LYS 1566	11.736 -3.842 27.563 1 00 35 3-
ATOM 71	1 CE LYS 1566	12.208 -5.279 27.459 1 00 55
3.000	<sup>2</sup> NZ LYS 1566	11.875 -6.001 28.747 1.00 25
3.000.	3 C LYS 1566	12.515 -7.421 28.716 1.00 32 83
7 Mote	O LYS 1566	13 756 25.623 1.00 29 92
Amos.	7567	11 700 20072 45.544 1.00 30 90
A moss	156/	12 422 24.979 1.00 30 67
3.0004	251 1367	13 136 24.138 1.00 28 44
ATOM 718 ATOM 719	721 126/	12.919 -0.225 1.00 27.19
ATOM 720	1268	14.011 1 731 22.395 1.00 25.36
ATOM 721	17014 17208	14.735 1.422 22.352 1.00 28.39
ATOM 722	CC 1568	15.188 2 600 21.130 1.00 28.41
	CG ASN 1568	16.396 3.350 20.418 1.00 30.32
CCCP /-		3.352 21.058 1.00 33.42





				17.418 2.720 21.317 1.00 35.16
ATOM	723 OD	1 ASN	1568	21.203 1.00 36.23
ATOM	724 ND	2 ASN	1568	2 442 21 314 1.00 20.54
MOTA	725 C	ASN	1568	16 479 0.373 22.388 1.00 30.67
	726 0	ASN	1568	20.244 1.00 27.65
ATOM	727 N	LEU	1569	1 270 20.247 1.00 29.10
ATOM	728 C	LEU	1569	17.203
ATOM	729 CI		1569	2 720 18 657 1.00 28.82
ATOM	730 C		1569	18.292
ATOM	, , , ,	D1 LEU	1569	18.236 -4.140 27.316 1.00 22.26
MOTA		D2 LEU	1569	17.994 -3.731 20 676 1 00 29.37
ATOM			1569	18.667 20.730 2013 1.00 29.72
ATOM				19.389 -1.525 22 1 00 30.89
MOTA				19.058 0.425 20.600 1.00 33.01
MOTA	,			20 374 0.943 20.121 1 00 30.95
MOTA		_		20.591 2.333 20 1 00 38.85
MOTA				21.896 2.983 20.584 1.00 43 63
MOTA		G ARC		21.968 4.472 20.303 2.00 53 34
MOTA		CD ARC		20.749 5.192 20.870 2.00
MOTA		VE AR		20.404 5.573 21.905 2.70
ATOM		CZ AR		21.184 5.310 22.933 1.00 59 53
MOTA	_	NH1 AR		19 272 6.252 22.000 1.00
MOTA	743	NH2 AR	·	20.475 0.947 22.229 1.00 33 93
MOTA	744	C AR		21,351 0.296 22.817 1.00 33 91
MOTA	745	O AR		1,639 72.865 1.00
ATOM	746	N GI		19.435 1.746 24.317 1.00 26 40
MOTA	747	CA GI		10 177 2.524 24.675 1.00 36.40
MOTA	748	CB GI		19 174 3.958 24.175 1.00 43.72
MOTA	749	CG GI		16 922 4 654 24 328
ATOM	750		LU 1571	15 793 3.959 24.322
ATOM	751	OE1 G		16 792 5.905 24.222 1.0
MOTA	752		LU 1571	19 380 0.361 24.955 1.5
MOTA	753	•	LU 1571	20 115 0.054 25.893 1.00
MOTA	754	-	LU 1571	19 503 -0.477 24.433 1.00
ATOM	755	• •	YR 1.572	10 234 -1.835 24.920 1.00 27.43
ATOM		CA T	YR 1572	17 387 -2.590 23.991 1.00 28.41
ATOM			YR 1572	37 196 -4.045 24.311 1.00 23.17
MOTA		CG 7	TYR 1572	16 224 -4.448 25.216 1.00 28.10
ATOM		CD1	TYR 1572	15 983 -5.784 25.456 1.00 28.32
ATOM		CE1 '	TYR 1572	17 936 -5.024 23.665 1.00 20.00
MOTA		CD2	TYR 1572	17 699 -6.361 23.899 1.00 22.20
MOTA		CE2	TYR 1572	16 721 -6.731 24.801 1.00 20.33
MOTA			TYR 1572	25 055 1.00 30.23
ATO			TYR 1572	24 960 1.00 30.90
ATO!			TYR 1572	2 223 25 901 1.00 30.68
OTA	· ·		TYR 1572	2 227 23.933 1.00 31.27
ATO!			LEU 1573	20.407
			LEU 1573	21.776 2 22.399 1.00 30.85
OTA OTA			LEU 1573	22.207 3 908 21.370 1.00 26.92
			LEU 1573	21.043
ATC			LEU 1573	5 272 21.695 1.00 25.82
OTA			LEU 1573	21.333
ATC			LEU 1573	22.801 -2.390 2-1 1 00 36.40
ATC		_	LEU 1573	00 5/4 -1.11/ 40
ATO	יו אוכ	-		

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	9/0/835		
ATOM	775	N	CLM
3	. •	**	GLN

A	TOM 77	-		
	ma	C - GIM	1574	22.815 -1.065 24.005
	701-	2 GDM	1574	23 763 24.88/ 1.00 37 25
	no	O THE	1574	23 722 25.759 1.00 37 41
	7014	ODIV	1574	24 240 25.522 1.00 38 07
		CD GTM	1574	24 046 2.329 24.147 1.00 40 76
		0774	1574	23 202 - 23.851 1.00 44 73
AT		01214	1574	24 606 2 24.597 1.00 46.47
AT		- 01114	1574	23 502 22.732 1.00 46 93
ATO	~	- GDM	1574	24 421 27.233 1.00 37 80
ATO	704	- AUM	1575	22 222 27.990 1.00 38 55
ATO		CA ALA	1575	27 046 0.732 27.617 1.00 37 20
ATC		CB ALA	15.75	20 304 21.021 28.987 1.00 35 47
ATO		C ALA	1575	22 102 - 29.178 1.00 31 42
ATO	• •	O ALA	1575	21 750 - 29.424 1.00 38 30
ATO		N ARG	1576	22 642 30.544 1.00 47 11
ATO	. 50	CA ARG	1576	22 942 28.528 1.00 37 59
ATO		CB ARG	1576	22 027 - 28.869 1.00 37 22
ATON		CG ARG	1576	20 500 - 28.111 1.00 36 82
ATOM		CD ARG	1.576	19 640 - 28.561 1.00 34 61
ATOM		NE ARG	576	18 300 - 27.640 1.00 31 82
ATOM		CZ ARG 1	576	17 500 7 28.201 1.00 37 54
ATOM	,	NH1 ARG 1	576	18 000 - 28.426 1.00 33 71
ATOM			576	76 227 5.055 28.149 1.00 33 60
ATOM	700		576	24 405 28,857 1,00 38 97
ATOM	600		576	24.790 -6 321 -683 1.00 38.53
ATOM	00-		57 <b>7</b>	25.226 -4.019 28.700 1.00 38.39
ATOM	000		577	26.661 4 105 28.538 1.00 39.28
ATOM			577	27.306 -2.055 28.394 1.00 39.33
ATOM			77	27.048 -2.402 26 52 1.00 35.44
ATOM	`		77	27.696 -1 043 20.384 1.00 33.45
ATOM		17 355	77	27.798 -0.747 24 907
ATOM		CI		28.284 0.385 24 304 3 5.69
ATOM		בר כער		28.719 1.359 25 175
ATOM	809 C			28.346 0.539 23 065
MOTA	810 O	12.0		27.222 -4.594 29 754
ATOM	811 N			26.652 -4.244 30 796 1 20 41.24
ATOM	812 CI			28.307 -5.381 29.760 1.00 41.03
ATOM	813 C			29.038 -6.041 28 667
ATOM	814 CE			20.8// -5.766 31.066 1.00
ATOM	815 CG		-	29.933 -6.809 30.686 1.00 40
ATOM	816 C	PRO 157		30.352 -6.391 29.327 1 00 45
ATOM	817 O	PRO 157		29.490 -4.493 31.672 1 00 45 5
ATOM	818 N	PRO 157		23.814 -3.538 30.947 1 00 44 7
ATOM	819 CD	PRO 1579		29.604 -4.432 33.003 1 00 45
ATOM	820 CA	PRO 1579		29.208 -5.463 33.981 1.00 46 36
ATOM ATOM	821 CB	PRO 1579		30.169 -3.265 33.685 1.00 47 56
ATOM	822 CG	PRO 1579		38.007 -3.708 35.141 1.00 46 45
ATOM	823 C	PRO 1579		31 575 1.00 47 51
ATOM	824 <sub>O</sub>	PRO 1579		33.403 33.200 1.00 50 19
ATOM	825 N	ALA 1592	,	19 002 33.196 1.00 53 53
:	826 CA	ALA 1592		20.535 5 076 32.478 1.00 60.30
				20.535 -5.076 32.445 1.00 59.47
000-				





**ATOM** 827 CB ALA 1592 20.975 -4.338 33.715 1.00 61.58 **ATOM** 828 С ALA 1592 21.367 -6.350 32.252 1.00 58.15 MOTA 829 0 ALA 1592 22.543 -6.285 31.879 1.00 59.09 **ATOM** B30 1.00 55.79 N ALA 1593 20.754 ..7.510 32.479 MOTA 831 CA ALA 1593 21.457 -8.775 32.324 1.00 55.06 **ATOM** 832 CB ALA 1593 20.519 -9.939 32.604 1.00 57.05 ATOM 833 С ALA 1593 22.053 -8.897 30.924 1.00 53.57 ATOM ALA 834 0 1593 21.402 -8.598 29.926 1.00 53.85 **ATOM** 835 N GLN 1594 23.303 -9.336 30.862 1.00 53.22 MOTA 836 CA GLN 1594 24.004 -9.490 29.599 1.00 50.13 **ATOM** 837 CB GLN 1594 25.400 -10.082 29.832 1.00 50.73 MOTA 838 CG GLN 1594 26.308 -9.253 30.743 1.00 54.69 **ATOM** 839 CD GLN 1594 27.550 -10.019 1.00 57.79 31.217 **ATOM** 840 OE1 GLN 1594 28.075 -10.900 30.524 1.00 58.82 ATOM 841 NE2 GLN 1594 28.026 -9.673 32.407 1.00 59.53 1594 ATOM 842 C GLN 23.210 -10.374 28.637 1.00 47.73 ATOM 843 0 GLN 1594 22.427 -11.241 29.054 1.00 47.09 ATOM 844 N LEU 1595 23.418 -10.133 27.350 1.00 45.64 **ATOM** 845 CA LEU 1595 22.758 -10.880 26.292 1.00 42.00 CB 22.405 -9.947 ATOM 846 LEU 1595 25.122 1.00 37.98 **ATOM** 847 CG LEU 1595 21.345 -8.894 25.446 1.00 37.70 **ATOM** 848 CD1 LEU 1595 21.568 .7.611 24.660 1.00 33.34 ATOM 849 CD2 LEU i.595 19.971 -9.479 25.222 1.00 32.84 ATOM 850 С LEU 23.729 -11.944 1595 25.828 1.00 40.92 ATOM 851 O LEU 1595 24.944 -11.745 25.855 1.00 41.12 ATOM 852 IJ SER 1596 25.471 23.201 -13.103 1.00 40.09 ATOM SER 853 CA 1596 24.044 -14.178 24.985 1.00 38.93 ATOM 854 CB SER 1596 23.388 -15.535 25.235 1.00 37.45 MOTA 855 OG SER 1596 22.158 -15.662 24.545 1.00 39.49 **ATOM** 856 C SER 1596 24.302 -13.987 23.499 1.00 39.41 ATOM 857 0 SER 1596 23.634 -13.183 22.832 1.00 39.51 ATOM 858 N SER 1597 25.266 -14.738 22.977 1.00 39.17 **ATOM** 859 CA SER 1597 25.587 -14.667 21.563 1.00 40.23 ATOM 860 CB SER 1597 26.740 -15.611 21.230 1.00 39.96 MOTA 861 ЭG SER 1597 27.865 -15.339 22.048 1.00 46.60 **ATOM** 862 3 SER 1597 24.347 -15.057 20.773 1.00 39.65 ATOM 863 0 SER 1597 24.066 -14.469 19.725 1.00 41.13 **ATOM** 864 N LYS 1598 23.590 -16.023 21.291 1.00 36.82 **ATOM** 865 CA LYS 1598 22.390 -16.467 20.611 1.00 36.17 ATOM 866 CB LYS 1598 21.827 -17.742 21.217 1.00 36.19 ATOM 867 CG LYS 1598 21.030 -18.562 20.180 1.00 39.59 MOTA 868 CD LYS 1598 20.150 -19.623 20.830 1.00 37.49 **ATOM** 869 LYS CE 1598 19.769 -20.719 19.855 1.00 39.64 ATOM 870 NZ LYS 1598 20.976 -21.437 19.380 1.00 41.43 ATOM 871 C LYS 1598 21.340 -15.381 20.649 1.00 37.72 ATOM 872 · O LYS 1598 20.604 -15.213 19.677 1.00 39.82 ATOM 873 N ASP 1599 21.291 -14.627 21.752 1.00 36.20 MOTA 874 CA ASP 1599 20.331 -13.530 21.907 1.00 33.96 **ATOM** 875 CB **ASP** 1599 20.456 -12.884 23.279 1.00 35.66 ATOM 876 CG **ASP** 1599 19.913 -13.744 24.394 1.00 36.18 **ATOM** 877 OD1 ASP 1599 20.365 -13.565 25.544 1.00 39.14

SSSD/55034. V01

878

OD2 ASP

1599

19.036 -14.593 24.128

1.00 33.40

ATOM





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AT	0,7	C ASP 1599	
AT		O ASP 1599	20.393 -12.471 20 857 1 22 -
ATO	-007	N LEU 1600	19.660 -11.953 20 325
ATO		C2	21.871 -12.123 20 706 1 22.80
ATO	OM 883		22.304 -11.121 19 725 1 2
ATC	M 884	20 1000	23.804 -10.850 19 916 1 22
ATO	M 885	CD2 1000	24.174 -10.153 21 242 1 20 5
ATO			25.660 -9.877 21 324 1 00 -
ATO	14	a	23.408 -8.857 21 369 1 00 -
ATO	м	220 1000	21.964 -11 502 1.00 21.94
OTA	M 889 M	7 1000	21 385 -10 724
ATON	v	1001	22,271 -12 764
ATON	4	1001	21.983 -12.260
ATOM		1001	22.648 -14 646
ATOM		G1 VAL 1601 G2 VAL 1601	22.403 -15 104
ATOM		- 7007	24.156 -14.550
ATOM	004	1001	20.474 -13 353 -1.00 29.92
ATOM	055 ()	1001	19.991 -13.142
ATOM	050 14		19.733 -13 500
ATOM	05, ()	1002	18.277 -12 (73
ATOM		K 1602	17.731 -14 250
ATOM	0	1002	16.317 -14 306
ATOM	900 C	SER 1602	17.669 -12 200 -18.646 1.00 35.77
ATOM	901 O	SER 1602	16.643 -12 74-
ATOM	000	CYS 1603	18.289 -11 262 16.465 1.00 25.13
ATOM	903 CA	CYS 1603	17.878 -9.073 1.00 26.09
ATOM	904 CB	CYS 1603	18.797 9 007
ATOM	905 SG	CYS 1603	18.512 7.705
ATOM	906 C	CYS 1603	17.994 -0.515
ATOM	907 0	CYS 1603	17 002 16.090 1.00 25.24
ATOM	908 N	ALA 1604	19.138 -9.054 15.520 1.00 27.48
ATOM	909 CA	ALA 1604	19.422 -9.502 1.00 26.80
ATOM	910 CB	ALA 1604	20.851 -10.025 14.073 1.00 26.15
ATOM	911 C	ALA 1604	18,419 -10,703 13,741 1,00 24,35
ATOM	912 0	ALA 1604	17.894 -0.712 13.168 1.00 26.61
ATOM	913 N	TYR 1605	18 130 -3.713 12.226 1.00 28.81
ATOM	914 CA	TYR 1605	17 175 13.488 1.00 27 10
ATOM	915 CB	TYR 1605	17 104 -2 12.730 1.00 27.02
ATOM	916 CG	TYR 1605	75 000 13.731 13.334 1.00 27 35
ATOM	917 CD1		16 100 17 12.789 1.00 31.67
ATOM		TYR 1605	15 060 15 11.546 1.00 32.96
ATOM	919 CD2	TYR 1605	14 830 14 722
ATOM	920 CE2	TYR 1605	13.520 1.00 31.42
	921 CZ	TYR 1605	13.038 1.00 28.20
ATOM	922 OH	TYR 1605	12 955 10.212 11.810 1.00 29.20
ATOM		TYR 1605	15 766 10.944 11.364 1.00 27.90
ATOM	924 0	TYR 1605	15 100 12.658 1.00 27.90
MOTA	925 N (	3LN 1606	15.180 -11.635 11.578 1.00 28 40
ATOM	926 CA 0	GLN 1606	13.231 -11.319 13.807 1.00 27.12
ATOM	000	GLN 1606	13.907 -10.699 13.892 1.00 25 32
ATOM	928 CG G	LN 1606	13.561 -10.383 15.342 1.00 24 31
ATOM	000	LN 1606	13.329 -11.608 16 210 1 -1
ATOM	930 OE1 G		13.052 -11.243 17.649 1 22
		2000	12.087 -10.542 17.944 1.00 26.11
SSSD/EFA:			20.11

ATOM	931	NE2	GLN	1606	13.917	-11.684	18.551	1.00 27.77
ATOM	932	С	GLN	1606	13.849	-9.415	13.078	1.00 27.52
MOTA	933	0	GLN	1606	12.825	-9.089	12.455	1.00 27.87
ATOM	934	N	VAL	1607	14.943	-8.662	13.122	1.00 27.90
MOTA	935	CA	VAL	1607	15.053	-7.419	12.359	1.00 26:41
MOTA	936	CB	VAL	1607	16.337	-6.661	12.731	1.00 25.61
ATOM	937	CG1	VAL	1607	16.545	-5.457	11.800	1.00 27.37
MOTA	938	CG2	VAL	1607	16.277	-6.224	14.190	1.00 21.50
ATOM	939	C	VAL	1607	15.035	-7.718	10.860	1.00 26.09
ATOM	940	0	VAL	1607	14.337	-7.046	10.096	1.00 28.48
ATOM	941	N	ALA	1608	15.795	-8.722	10.435	1.00 23.05
ATOM	942	CA	ALA	1608	15.812	-9.079	9.027	1.00 20.32
ATOM	943	CB	ALA	1608	16.823	-10.145	8.783	1.00 14.95
ATOM	944	C	ALA	1608	14.418	-9.558	8.600	1.00 23.08
ATOM	945	0	ALA	1608	14.033	-9.405	7.432	1.00 23.91
ATOM	946	N	ARG	1609	13.671	-10.169	9.530	1.00 24.57
ATOM	947	CA	ARG	1609	12.314	-10.628	9.246	1.00 24.30
ATOM	948	CB	ARG	1609	11.822	-11.577	10.326	1.00 26.13
ATOM	949	CG	ARG	1609	12.278	-12.979	10.114	1.00 31.07
ATOM	950	CD	ARG	1609	11.449	-13.885	10.939	1.00 36.13
ATOM	951	NE	ARG	1609	10.771	-14.865	10.115	1.00 38.37
ATOM	952	CZ	ARG	1609	9.931	-15.778	10.594	1.00 37.95
ATOM	953	NHl	ARG	1609	9.674	-15.828	11.898	1.00 35.31
ATOM	954	NH2	ARG	1609	9.353	-16.649	9.776	1.00 37.85
ATOM	955	С	ARG	1609	11.318	-9.490	9.065	1.00 22.34
ATOM	956	0	ARG	1609	10.470	-9.542	8.160	1:00 24.57
ATOM	957	N	GLY	1610	11.375	-8.500	9.948	1.00 20.52
ATOM	958	CA	GLY	1610	10.497	-7.353	9.827	1.00 19.33
ATOM	959	C	GLY	1610	10.732	-6.715	8.464	1.00 20.04
MOTA	960	0	GLY	1610	9.794	-6.455	7.693	1.00 19.10
ATOM	961	N	MET	1611	12.011	-6.545	8.130	1.00 18.21
MOTA	962	CA	MET	1611	12.423	-5.970	6.851	1.00 20.32
ATOM	963	CB	MET	1611	13.925	-5.737	6.838	1.00 19.20
MOTA	964	CG	MET	1611	14.371	-4.547	7.694	1.00 20.83
MOTA	965	SD	MET	1611	13.449	-2.960	7.422	1.00 25.39
MOTA	966	CE	MET	1611	13.869	-2.525	5.757	1.00 18.67
ATOM	967	C	MET	1611	12.024	-6.843	5.670	1.00 23.98
ATOM	968	0	MET	1611	11.608	-6.332	4.613	1.00 24.13
ATOM	969	N	GLU	1612	12.141	-8.162	5.825	1.00 25.76
ATOM	970	CA	GLU	1612	11.759	-9.059	4.743	1.00 25.49
ATOM	971	CB	GLU	1612	11.980	-10.522	5.110	1.00 26.09
ATOM	972	CG	GLU	1612	11.587	-11.468	3.968	1.00 26.56
ATOM	973	CD	GLU	1612	11.735	-12.942	4.313	1.00 29.26
ATOM	974	OE1	GLU	1612	11.386	-13.316	5.448	1.00 29.10
ATOM	975	OE2	GLU	1612	12.190	-13.725	3.443	1.00 31.11
ATOM	976	С	GLU	1612	10.283	-8.821	4.398	1.00 26.29
ATOM	977	0	GLU	1612	9.916	-8.728	3.226	1.00 28.46
MOTA	978	N	TYR	1613	9.437	-8.700	5.422	1.00 24.78
MOTA	979	CA	TYR	1613	8.003	-8.456	5.212	1.00 23.07
MOTA	980	CB	TYR	1613	7.263	-8.526	6.549	1.00 23.75
MOTA	981	CG	TYR	1613	5.785	-8.218	6.449	1.00 20.80
ATOM	982	CD1	TYR	1613	4.880	-9.213	6.062	1.00 20.97

3.00					
ATO		983	CE1	TYR 1613	3.517 ~8.944 5.958 1.00 20 03
ATO		984		TYR 1613	5.330 1.00 20.03
ATC		985		TYR 1613	3 926 6 66
ATC ATC	_	986		YR 1613	3 046 2 55
ATO		987		YR 1613	1 694 7 100 24.87
ATO		88	_	YR 1613	7 766 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ATO		89		YR 1613	5 970 6 970
ATO			_	EU 1614	8 436
ATO				EU 1614	8 321 4 722
ATO				EU 1614	9 160 2 7.5
ATO				EU 1614	9 607 3 7 7 7 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ATO			CD1 L		9 504 2 10-
MOTA			CD2 LI	_	7.230 -2.705
ATOM			L		9 720
ATOM			) LE		9 073
ATOM					9 810 5 22.25
ATOM			A AL		10 313 5 105
ATOM		_	B AL		11 625 6 20.52
ATOM			-		9 264 6 222 1.00 19.78
ATOM					9 945 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
ATOM					P 602
ATOM	100		A SE		7 660 7 650
ATOM	100				7 282 0 215
ATOM	100	_			6.415 -8.966 2.007 1.00 15.96
ATOM	1008	_	SEI		6.397 -7.062 -0.018 1.00 22.05
ATOM	1009	_	SEF		5.650 -7.266 -0.975 1 00 22 62
ATOM	1010		LYS		6.136 -6.135 0.895 1.00 23.32
ATOM	1011				4.997 -5.237 0.779 1 00 23 03
ATOM	1012				4.436 -4.881 2.160 1.00 21.50
ATOM	1013				3.709 -6.046 2.851 1.00 34.04
ATOM	1014				2.463 -6.448 2.059 1.00 26 57
ATOM	1015			1617 1617	1.691 -7.571 2.725 1.00 31.05
ATOM	1016		LYS	1617	2.401 -8.852 2.601 1.00 38 73
ATOM	1017	0	LYS	1617	3.346 -3.981 -0.017 1.00 24.01
ATOM	1018	N	LYS	1618	4.308 -3.007 -0.013 1.00 28 15
ATOM	1019	CA	LYS	1618	0.456 -4.002 -0.679 1.00 23 84
ATOM	1020	CB	LYS	1618	0.957 -2.883 -1.528 1.00 24 05
MOTA	1021	CG	LYS	1618	5.871 -2.513 -2.555 1.00 25.74
ATOM	1022	CD	LYS	1618	3.734 -3.465 -3.749 1.00 28.34
MOTA	1023	CE	LYS	1618	3.337 -4.914 -3.328 1.00 32.45
ATOM	1024	NZ	LYS	1618	4.373 -4.520 1.00 30.41
ATOM	1025	C	LYS	1618	7 404 -5.354 1.00 31.84
ATOM	1026	0	LYS	1618	7.404 -1.610 -0.796 1.00 23.84
MOTA	1027	N	CYS	1619	7.533 -0.548 -1.402 1.00 20.60
ATOM	1028	CA	CYS	1619	7.719 -1.744 0.489 1.00 25.11
ATOM	1029	CB	CYS	1619	7 333 -0.614 1.312 1.00 21.68
ATOM	1030	SG	CYS	1619	7.338 -0.690 2.643 1.00 20.84
ATOM	1031	C	CYS	1619	7.916 0.427 3.957 1.00 26.69
ATOM	1032	O	CYS	1619	10 257 1 107
ATOM	1033	N	ILE	1620	10.257 -1.435 1.958 1.00 25.60
ATOM	1034	CA	ILE	1620	10.110 0.717 1.288 1.00 23.91
					11.532 1.046 1.474 1.00 26.01
					•

MOTA	1035	CB	ILE	1620	12.098	1.830	0.236	1.00	22.61
ATOM	1036	CG2	ILE	1620	13.551	2.259	0.471	1.00	16.86
ATOM	1037	CG1	ILE	1620	12.014	0.977	-1.026	1.00	22.72
ATOM	1038	CD1	ILE	1620	12.096	1.804	-2.316	1.00	23.62
ATOM	1039	C	ILE	1620	11.566	1.934	2.729	1.00	26.83
ATOM	1040	О	ILE	1620	10.900	2.965	2.772		28.92
ATOM	1041	N	HIS	1621	12.293	1.500	3.758		26.44
ATOM	1042	CA	HIS	1621	12.386	2.245	5.007		23.61
ATOM	1043	СВ	HIS	1621	13.142	1.429	6.065		20.98
ATOM	1044	CG	HIS	1621	12.940	1.917	7.463		21.57
ATOM	1045		HIS	1621	12.321	1.346	8.528		20.74
ATOM	1046		HIS	1621	13.382	3.151	7.897		21.08
ATOM	1047		HIS	1621	13.035	3.321	9.162		21.00
ATOM	1048	NE2		1621	12.396	2.237	9.572		21.97
ATOM	1049	C	HIS	1621	13.054	3.582	4.841		24.83
ATOM	1050	0	HIS	1621	12.560	4.585	5.310		25.76
ATOM	1051	N	ARG	1622	14.247	3.565	4.269		27.57
ATOM	1052	CA	ARG	1622	15.056	4.776	4.066		26.47
ATOM	1053	СВ	ARG	1622	14.233	5.918	3.460		20.08
ATOM	1054	CG	ARG	1622	13.762	5.634	2.077		15.87
ATOM	1055	CD	ARG	1622	12.998	6.791	1.501		11.86
ATOM	1056	NE	ARG	1622	12.613	6.458	0.144		12.46
ATOM	1057	CZ	ARG	1622	11.537	5.748	-0.178		11.18
ATOM	1058		ARG	1622	10.711	5.304	0.767	0.50	7.16
ATOM.	1059		ARG	1622	11.340	5.398	-1.442	0.50	9.57
ATOM	1060	C	ARG	1622	15.813	5.250	5.325		26.18
ATOM	1061	0	ARG	1622	16.645	6.150	5.250		26.90
ATOM	1062	N	ASP	1623	15.544	4.650	6.480		27.26
ATOM	1063	CA	ASP	1623	16.268	5.042	7.684		29.80
ATOM	1064	CB	ASP	1623	15.714	6.330	8.292		32.13
ATOM	1065	CG	ASP	1623	16.690	6.940	9.298		37.87
MOTA	1066	OD1	ASP	1623	16.237	7.671	10.202		42.95
ATOM	1067	OD2	ASP	1623	17.907	6.684	9.191	1.00	41.09
ATOM	1068	С	ASP	1623	16.364	3.943	8.738		29.10
ATOM	1069	0	ASP	1623	16.164	4.168	9.939		27.69
ATOM	1070	N	LEU	1624	16.723	2.755	8.270	1.00	28.23
MOTA	1071	CA	LEU	1624	16.874	1.599	9.129	1.00	26.00
ATOM	1072	CB	LEU	1624	16.944	0.351	8.245	1.00	22.14
ATOM	1073	CG	LEU	1624	17.036	-0.998	8.941	1.00	22.32
ATOM	1074	CD1	LEU	1624	15.853	-1.196	9.932	1.00	17.01
MOTA	1075	CD2	LEU	1624	17.068	-2.064	7.848	1.00	20.50
ATOM	1076	C	LEU	1624	18.129	1.757	10.003	1.00	25.89
MOTA	1077	0	LEU	1624	19.247	1.917	9.499	1.00	
MOTA	1078	N	ALA	1625	17.930	1.706	11.316	1.00	25.58
MOTA	1079	CA	ALA	1625	19.006	1.864	12.292	1.00	23.16
MOTA	1080	CB	ALA	1625	19.323	3.340	12.493	1.00	19.06
ATOM	1081	С	ALA	1625	18.475	1.286	13.584	1.00	24.12
ATOM	1082	0	ALA	1625	17.269	1.083	13.721	1.00	
ATOM	1083	N	ALA	1626	19.357	1.041	14.543	1.00	
ATOM	1084	CA	ALA	1626	18.929	0.491	15.827	1.00	25.07
ATOM	1085	CB	ALA	1626	20.148	0.145	16.691	1.00	
ATOM	1086	C	ALA	1626	18.015	1.474	16.560	1.00	

ATO		87 (	C (	<b>L</b> A	1626	17 1	104 -						
ATO		88 1		<b>I</b> RG	1627	17.1 18.1		.069	17.3		00	26.3	38
ATC			CA A	LRG	1627	17.3		.770	16.3	08 1	.00	23.0	80
ATO		90 (	B A	RG	1627	17.8		.784	16.9		.00	24.0	)5
ATO		_	G A	RG	1627	17.7		.187	16.5			28.0	
ATO			D A	RG	1627	18.1		.501	15.0			37.5	
ATO.			E A	RG	1627	18.4		920	14.74		.00	42.1	0
ATO		-		RG	1627	19.6		085	13.31		.00	42.6	7
ATO			H1 A		1627	20.7		006	12.78		. 00	43.5	8
ATO			H2 A	RG	1627	19.84		752 201	13.56			46.1	
ATO		_	A	₹G	1627	15.92		632	11.49		.00	43.7	8
ATON	_	_	A	RG	1627	15.01		979	16.48			23.04	
ATON	_		AS	SN	1628	15.72		979 093	17.21			22.27	
ATOM			A AS		1628	14.38		934	15.28			24.49	
ATOM	_			N	1628	14.35		934 407	14.72			23.80	
ATOM ATOM					1628	14.50		918	13.26		00 2	27.82	?
ATOM			1 AS		1628	13.87		586	13.14		00 3	0.25	,
ATOM			2 AS	N :	1628	15.36			13.86		00 3	2.33	
ATOM		_	AS		1628	13.78			12.220		00 3	1.50	
ATOM			AS:	N :	1628	12.89			14.833		JO 2	3.93	
ATOM	,		VA:	-	1629	14.30			14.056 15.763			3.64	
ATOM					629	13.778			16.036		_	4.10	
ATOM	1109		VAI		.629	14.829			15.823		10 2	2.59	
ATOM	1110 1111		l VAI		629	14.346			16.462		10 2	1.16	
ATOM	1112		VAI		629	15.068			14.341		10 T	7.53	
ATOM	1113	C	VAI		629	13.411	-0.5		17.520		0 14		
ATOM	1114	0	VAL	_	629	14.237	-0.2		L8.357		0 24		
ATOM	1115	N	LEU		630	12.181			7.850		0 24 0 24		
ATOM	1116	CA CB	LEU	_	630	11.751	-0.9		9.239	1.0	0 26	- 54	
ATOM	1117	CG	LEU	_	630	10.447	-0.12		9.359	1.0	0 26	1.53	
ATOM	1118		LEU LEU		530	10.522	1.29		8.758	1.0	0 24	.13	
ATOM	1119		LEU		530	9.149	1.87		8.601		0 20		
MOTA	1120	C	LEU		530	11.339	2.19		9.618	1.00		.77	
ATOM	1121	ō	LEU		30	11.641	-2.32	7 1	9.835		28		
ATOM	1122	N	VAL		330 31	11.475	-3.32	0 1	9.108	1.00		.31	
ATOM	1123	CA	VAL		31	11.792	-2.41		1.153	1.00	_	.21	
ATOM	1124	CB	VAL		31	11.741	-3.69		1.866	1.00	26	. 96	
ATOM	1125		VAL	16		13.068	-3.93		2.624	1.00	25	.71	
ATOM	1126	CG2		16			-5.34		3.222	1.00			
ATOM	1127	C	VAL	16		14.240	-3.68	9 21	1.680	1.00			
ATOM	1128	0	VAL	16		10.560	-3.75		8.836	1.00	29.	84	
ATOM	1129	N	THR	16:		10.419	-2.918		.738	1.00	32.	46	
ATOM	1130		THR	16:		9.703	-4.756		.641	1.00			
MOTA	1131		THR	16:		8.530	-4.939		.487	1.00	31.	16	
ATOM	1132	OG1		163		7.476	-5.800		.793	1.00			
MOTA	1133		THR	163		7.948	-7.152		.708	1.00	29.	17	
ATOM			THR	163		7.186	-5.262		.414	1.00	22.	23	
ATOM	1135		THR	163		8.882	-5.603		.809	1.00			
MOTA	1136		GLU	163		9.950	-6.185		.946	1.00	33.	23	
MOTA	1137		3LU	163		7.946	-5.589		.751	1.00	34.	38	
MOTA	1138		GLU	163		8.165 6.881	-6.193		. 062	1.00	35.5	51	
				_		0.001	-6.114	27.	.899	1.00	35.4	18	

ATOM	1139	CG	GLU	1633	7.004	-6.685	29.309	1.00	45.16
ATOM	1140	CD	GLU	1633	8.070	-5.999	30.183	1.00	50.45
MOTA	1141	OE1	GLU	1633	8.174	-4.750	30.163	1.00	52.70
MOTA	1142		GLU	1633	8.789	-6.723	30.919	1.00	53.59
MOTA	1143	C	GLU	1633	8.624	-7.635	26.930	1.00	35.40
ATOM	1144	0	GLU	1633	9.387	-8.119	27.758	1.00	36.57
ATOM	1145	N	ASP	1634	8.204	-8.308	25.861	1.00	36.76
ATOM	1146	CA	ASP	1634	8.573	-9.709	25.662	1.00	37.95
MOTA	1147	CB	ASP	1634	7.435	-10.491	24.991	1.00	42.90
MOTA	1148	CG	ASP	1634	6.100	-10.315	25.706	1.00	49.06
MOTA	1149		ASP	1634	5.885	-10.957	26.759	1.00	50.95
MOTA	1150		ASP	1634	5.256	-9.544	25.197	1.00	53.92
MOTA	1151	С	ASP	1634	9.842	-9.882	24.840	1.00	36.05
ATOM	1152	0	ASP	1634	10.148	-10.988	24.414	1.00	34.95
ATOM	1153	N	ASN	1635	10.582	-8.787	24.655	1.00	36.53
MOTA	1154	CA	ASN	1635	11.833	-8.763	23.868	1.00	36.21
ATOM	1155	CB	ASN	1635	12.893	-9.692	24.471	1.00	37.91
ATOM	1156	CG	ASN	1635	13.335	-9.244	25.840	1.00	37.60
ATOM	1157	OD1	ASN	1635	13.496	-8.057	26.088	1.00	42.72
ATOM	1158	ND2	ASN	1635	13.525	-10.191	26.743	1.00	38.03
ATOM	1159	С	ASN	1635	11.641	-9.073	22.372	1.00	34.59
MOTA	1160	0	ASN	1635	12.431	-9.799	21.754	1.00	33.52
MOTA	1161	N	VAL	1636	10.557	-8.541	21.819	1.00	31.95
ATOM	1162	CA	VAL	1636	10.260	-8.722	20.415	1.00	28.92
ATOM	1163	CB	VAL	1636	8.743	-8.945	20.177	1.00	31.00
ATOM	1164	CG1	VAL	1636	8.451	-9.066	18.678	1.00	29.52
ATOM	1165	CG2	VAL	1636	8.289	-10.220	20.884	1.00	29.03
ATOM	1166	С	VAL	1636	10.725	-7.461	19.721	1.00	28.05
ATOM	1167	0	VAL	1636	10.432	-6.355	20.179	1.00	25.21
MOTA	1168	И	MET	1637	. 11.567	-7.637	18.707	1.00	28.78
ATOM	1169	CA	MET	1637	12.107	-6.539	17.927	1.00	27.29
ATOM	1170	CB	MET	1637	13.325	-7.008.	17.138	1.00	27.97
ATOM	1171	CG	MET	1637	14.446	-7.576	17.982	1.00	29.31
ATOM	1172	SD	MET	1637	15.051	-6.440	19.245	1.00	29.58
ATOM	1173	CE	MET	1637	15.163	-7.542	20.648	1.00	23.51
ATOM	1174	С	MET	1637	11.033	-6.108	16.951	1.00	26.60
ATOM	1175	0	MET	1637	10.479	-6.951	16.244	1.00	26.60
ATOM	1176	N	LYS	1638	10.758	-4.805	16.893	1.00	24.35
ATOM	1177	CA	LYS	1638	9.745	-4.255	16.006	1.00	20.79
MOTA	1178	CB	LYS	1638	8.495	-3.883	16.793	1.00	
ATOM	1179	CG	LYS	1638	7.723	-5.087	17.268	1.00	22.82
ATOM	1180	CD	LYS	1638	6.442	-4.699	17.969	1.00	
MOTA	1181	CE	LYS	1638	5.560	-5.934	18.189	1.00	
ATOM	1182	NZ	LYS	1638	4.892	-6.414	16.941	1.00	
ATOM	1183	С	LYS	1638	10.254	-3.034	15.257	1.00	22.79
ATOM	1184	0	LYS	1638	10.613	-2.041	15.868	1.00	
ATOM	1185	N	ILE	1639	10.259	-3.101	13.934	1.00	
ATOM	1186	CA	ILE	1639	10.707	-1.984	13.113	1.00	
ATOM	1187	CB	ILE	1639	10.925	-2.439	11.648	1.00	
ATOM	1188		ILE	1639	11.270	-1.262	10.766	1.00	
ATOM	1189		ILE	1639	12.068	-3.454	11.604	1.00	
ATOM	1190	CD1	ILE	1639	11.975	-4.369	10.461	1.00	26.92

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86	-0.846	13.173	1.00 25.63	

			•	
	OM 119:	l C	ILE 1639	9.686 -0.846 13.173 1.00
	'OM 1192	2 0	ILE 1639	9 1000 -0.846 13.173 1.00 25.63
AT		N	ALA 1640	10.205 21.075 13.042 1.00 26.20
AT		CA	ALA 1640	0.364 13.390 1.00 27.31
AT		CB	ALA 1640	1.577 13.497 1.00 27 45
ATO	OM 1196	C	ALA 1640	2.211 14.862 1.00 27 20
ATO		0	ALA 1640	2.595 12.411 1.00 27 87
ATO			ASP 1641	10.765 2.522 11.755 1.00 26 27
ATC		_		8.815 3.551 12.237 1 00 20 66
ATC	M 1200	_		8.952 4.631 11.259 1.00 21.55
ATO				10.096 5.581 11 646 1 00 33
ATO		OD1		9.713 6.551 12.771 1.00 33.40
ATO		OD2	_	10.475 7.524 12 953 1 00 25
ATO				8.684 6.355 13.470 1.00 22 25
ATO			_	9 080 4 335
ATO			SP 1641	9 526 5 000
ATON	_		HE 1642	8 611 7 020
ATON	,		HE 1642	8 664 2 700
ATOM			HE 1642	8 459 1 200
ATOM	05	CG P	HE 1642	7 167 0 555
ATOM		CD1 P		6 002 0 545
ATOM		CD2 p		7 119 0 7.542 1.00 22.76
ATOM		CE1 P		4 796 0 004
ATOM		CE2 P		5 926 0 244
ATOM		CZ PI	IE 1642	4 760 0 250
ATOM		C PF	IE 1642	7 686 3 349
ATOM		O PH	E 1642	7 946 3 336
ATOM		N GL	Y 1643	6 600 3 70-
ATOM		CA GL	Y 1643	5 640 4 17 1.00 30.42
		C GL		5 736 5 000
ATOM		O GL	Y 1643	4 896 6 707
ATOM		N LE	U 1644	6.816 6.47
ATOM		CA LE	U 1644	7 077 7 000 1.00 31.65
ATOM		CB LE	U 1644	8 363 0 000 1.00 36.03
ATOM		G LE		B 321 0 222 1.00 32.41
ATOM		D1 LEC	J 1644	9.446 1.00 35.30
ATOM		D2 LEU		0.62/ 10.384 1.00 37.60
ATOM	1227 C	LEU		3.186 10.190 1.00 36.62
ATOM	1228 O	LEU		7.770 8.708 6.293 1.00 40.21
ATOM	1229 N	ALA		5.312 1.00 40 55
ATOM	1230 C	A ALA	1645	6.293 1.00 44.50
ATOM	1231 C			5.1331 10.786 5.148 1.00 48.66
ATOM	1232 C	ALA		3.432 11.762 5.241 1.00 45.63
ATOM	1233 0	ALA		5.173 1.00 51.32
ATOM	1234 N	ALA		6.163 1.00 52 6B
ATOM	1235 C		1646	0.727 11.444 4.107 1.00 52 77
ATOM	1236 CE		1646	10.023 12.121 4.077 1.00 54 73
ATOM	1237 C	ALA	1646	11.108 11.194 4.646 1.00 55 74
ATOM	1238 O	ALA	1646	10.446 12.601 2.692 1 00 56 41
ATOM	1239 N	ASP		10.430 11.823 1.740 1.00 57 76
ATOM	1240 CA		1647	10.811 13.876 2.567 1.00 58 30
ATOM	1241 CB		1647	11.280 14.394 1.283 1.00 50 55
ATOM	1242 CG		1647	10.898 15.861 1 083 1 00 50
	0	ASP	1647	11.128 16.339 -0.356 1.00 60.67
				1.00 60.67

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**ATOM** 1243 OD1 ASP 1647 12.110 15.908 -1.009 1.00 61.21 MOTA 1244 OD2 ASP 1647 10.337 17.173 -0.835 1.00 61.34 MOTA 1245 С ASP 1647 12.793 14.236 1.273 1.00 60.16 **ATOM** 1246 0 ASP 1647 13.523 15.023 1.889 1.00 58.16 MOTA 1247 N ILE 1648 13.248 13.209 0.562 1.00 61.28 MOTA 1248 CA ILE 1648 14.658 12.878 0.439 1.00 62.12 **ATOM** 1249 CB ILE 1648 14.848 11.626 -0.444 1.00 59.97 **ATOM** 1250 CG2 ILE 1648 14.023 10.469 0.131 1.00 58.26 CG1 ILE MOTA 1251 1648 14.429 11.922 -1.883 1.00 55.69 MOTA 1252 CD1 ILE 1648 15.005 10.976 -2.890 1.00 54.38 **ATOM** 1253 С ILE 1648 15.470 14.047 -0.127 1.00 65.02 MOTA 1254 0 ILE 1648 16.633 14.245 0.233 1.00 66.85 MOTA 1255 N HIS 1649 14.844 14.839 -0.995 1.00 65.85 **ATOM** 1256 CA HIS 1649 15.505 15.992 -1.589 1.00 66.73 MOTA 1257 HIS CB 1649 14.859 16.358 -2.934 1.00 65.67 MOTA 1258 CG HIS 1649 15.142 15.388 -4.038 1.00 66.47 ATOM 1259 CD2 HIS 1649 16.253 14.686 1.00 67.11 -4.355 ATOM 1260 ND1 HIS 1649 14.210 15.064 -4.999 1.00 65.21 ATOM 1261 CE1 HIS 1649 14.733 14.216 -5.867 1.00 66.52 MOTA 1262 NE2 HIS 1649 13.966 15.974 -5.494 1.00 66.25 MOTA 1263 C HIS 1649 15.505 17.200 -0.663 1.00 68.55 MOTA 1264 0 HIS 1649 15.636 1.00 69.35 18.341 -1.116 MOTA 1265 N HIS 1650 15.273 16.963 0.629 1.00 71.25 ATOM 1266 CA HIS 1650 15.262 18.026 1.633 1.00 73.53 **ATOM** 1267 CB HIS 1650 13.849 18.551 1.860 1.00 76.79 ATOM 1268 CG HIS 1650 13.342 19.448 0.765 1.00 83.36 **ATOM** 1269 CD2 HIS 1650 13.509 20.772 0.537 1.00 86.47 MOTA 1270 ND1 HIS 1650 12.571 18.984 -0.270 1.00 87.02 MOTA 1271 CE1 HIS 1650 12.279 19.983 -1.076 1.00 88.66 MOTA 1272 NE2 HIS 1650 12.840 21.080 -0.609 1.00 88.34 MOTA 1273 C HIS 1650 15.872 17.580 2.965 1.00 73.11 **ATOM** 1274 0 HIS 1650 15.686 18.241 3.977 1.00 73.23 **ATOM** 1275 N ILE 1651 16.599 16.464 2.949 1.00 72.64 MOTA 1276 CA ILE 1651 17.234 15.937 4.143 1.00 72.54 MOTA 1277 CB ILE 1651 17.660 14.472 3.942 1.00 74.59 MOTA 1278 CG2 ILE 1651 18.463 13.966 5.142 1.00 75.52 ATOM 1279 CG1 ILE 1651 16.426 13.591 3.752 1.00 77.59 MOTA 1280 CD1 ILE 1651 16.747 12.141 3.472 1.00 80.12 MOTA 1281 С ILE 1651 18.463 16.769 4.523 1.00 71.47 ATOM 1282 0 ILE 1651 19.326 17.022 3.688 1.00 72.40 MOTA 1283 N ASP 1652 18.529 17.197 5.784 1.00 70.34 ATOM 1284 ASP CA 1652 19.678 17.976 6.235 1.00 68.57 MOTA 1285 CB ASP 1652 19.272 18.878 7.411 1.00 72.80 **ATOM** 1286 ASP CG 1652 20.456 19.640 7.982 1.00 76.90 **ATOM** 1287 OD1 ASP 1652 21.463 19.888 7.287 1.00 79.62 **ATOM** 1288 OD2 ASP 1652 20.369 20.030 9.170 1.00 80.36 ATOM 1289 C ASP 1652 20.771 17.007 6.652 1.00 66.01 ATOM 1290 0 **ASP** 1652 20.709 16.421 1.00 64.75 7.735 **ATOM** 1291 1653 N TYR 21.778 16.868 5.808 1.00 64.05 **ATOM** 1292 CA TYR 1653 22.906 15.978 6.074 1.00 63.55 ATOM 1293 CB TYR 1653 23.829 15.913 4.855 1.00 63.81 **ATOM** TYR 1294 CG 1653 23.316 14.993 3.771 1.00 65.65

A.	TOM	1295	CD1	TYR	1653					
A		1296	CE1			24.0		4.710	2.643	1.00 65.32
An		1297	CD2		1653	23.6		3.810	1.674	
		1298			1653	22.0		.357	3.903	
		.299		TYR	1653	21.6		.451	2.940	
		300	CZ	TYR	1653	22.4		.182		
AT				TYR	1653	21.9		. 272	1.833	1.00 70.13
AT	_	301	_	TYR	1653	23.7		.334	0.902	1.00 72.73
ATO		302		TYR	1653	24.3			7.328	1.00 62.96
		303	N '	TYR	1654	23.6		.473	7.938	1.00 63.31
ATO		304	CA '	ΓΥR	1654	24.3		.598	7.727	1.00 63.02
ATO		305	CB ?	ryr '	1654			.065	8.902	1.00 63.89
ATC		306		YR	1654	24.89		.491	8.684	1.00 60.37
ATC		307	CD1 1	YR	1654	26.01		565	7.669	1.00 59.33
ATC	DM 13	808		YR	1654	25.73		673	6.313	1.00 59.29
ATO		109			1654	26.75		687	5.362	1.00 61.50
ATO		10	_		1654	27.34			8.061	1.00 60.05
ATO.	M 13					28.38			7.119	1 00 61 0-
ATO					1654	28.08	2 19.		5.773	1.00 61.35
ATO					1654	29.09	8 19.		4.842	1.00 62.41
ATO			_		1654	23.586	6 17.		0.192	1.00 60.57
ATOM					L654	24.104	1 18.		1.252	1.00 65.65
ATON			1 L		.655	22.349	17.			1.00 67.31
ATOM			CA LY		.655	21.499	17.		).118	1.00 67.52
ATOM		`	B Ly		655	20.028	17.4		303	1.00 69.54
ATOM	_		G LY		655	19.057			.893	1.00 71.09
ATOM		_	D LY	_	655	17.648			.049	1.00 73.08
ATOM	_	-	E LY	S 1	655	16.624			.531	1.00 76.73
ATOM				S 1	655	15.232			.568	1.00 81.94
		_	LY	S 1	655	21.783			.072	1.00 84.53
ATOM			LY.		555	21.952			.076 ]	1.00 70.33
ATOM			LY		556	. 21.825	15.0		.478 1	00 70.43
ATOM	132	5 C	A LYS		556	22.093	16.2		403 1	.00 70.11
ATOM	132		LYS		56		15.0		274 1	.00 70.03
ATOM	132	7 C	LYS		56	23.049	15.48		394 1	.00 67.72
ATOM	1328	GI CI			56	24.473	15.71		947 1	.00 66.34
ATOM	1329	CE			56	25.326	16.12		136 1	.00 66.60
ATOM	1330				56	26.801	15.83	9 15.		.00 64.71
ATOM	1331	. С	LYS			27.612	16.05	9 17.		.00 62.24
ATOM	1332		LYS			20.823	14.48	0 14.		.00 70.67
ATOM	1333		THR			19.759	15.10	4 14.		.00 71.91
ATOM	1334		THR	16:		20.941	13.26	5 15.		00 69.38
ATOM	1335		THR	16		19.818	12.58	6 16.0		00 69.38
ATOM	1336		THR	169		20.052	11.05	1 16.1		00 68.30
ATOM	1337	CC	TILK	169		21.179	10.75	7 16.9		00 69.30
ATOM	1338		THR	165		20.310	10.47			00 68.20
ATOM	1339	С	THR	165		19.706	13.145			00 69.71
ATOM		0	THR	165		20.521	13.971			00 67.60
ATOM	1340	N	ALA	165			12.694			00 67.40
	1341	CA	ALA	165	8	30				00 67.83
ATOM	1342	CB	ALA	165			13.163	• •		00 67.73
ATOM	1343	C	ALA	165			12.503		34 1.(	00 68.87
ATOM	1344	0	ALA	165		20 25-	12.820	-	64 1.(	00 66.59
ATOM	1345	N	ASN	165			13.640		15 1.0	00 66.33
ATOM	1346	CA	ASN	165			11.616		29 1.C	00 65.38
					-	21.545	11.143	20.80	1.0	0 62.65

ATOM	1347	CB	ASN	1659	21.702	9.638	20.616	1.00	63.61
ATOM	1348	CG	ASN	1659	22.548	9.009	21.697		64.09
ATOM	1349		ASN	1659	22.526	9.451	22.850	1.00	63.69
ATOM	1350		NSA	1659	23.279	7.959	21.345	1.00	64.10
MOTA	1351	С	ASN	1659	22.808	11.844	20.321	1.00	60.46
MOTA	1352	0	ASN	1659	23.882	11.601	20.856	1.00	60.78
MOTA	1353	N	GLY	1660	22.671	12.675	19.285	1.00	58.84
ATOM	1354	CA	GLY	1660	23.803	13.407	18.735	1.00	56.69
ATOM	1355	C	GLY	1660	24.570	12.721	17.616	1.00	56.40
MOTA	1356	0	GLY	1660	25.738	13.028	17.377	1.00	56.43
MOTA	1357	N	ARG	1661	23.929	11.779	16.937	1.00	56.00
ATOM	1358	CA	ARG	1661	24.585	11.048	15.849	1.00	53.80
ATOM	1359	CB	ARG	1661	24.312	9.540	15.952	1.00	54.52
MOTA	1360	CG	ARG	1661	24.876	8.879	17.218	1.00	55.28
MOTA	1361	CD	ARG	1661	24.556	7.395	17.226	1.00	58.01
MOTA	1362	NE	ARG	1661	25.051	6.670	18.396	1.00	58.41
MOTA	1363	CZ	ARG	1661	24.918	5.355	18.559		59.08
ATOM	1364	NH1		1661	24.306	4.637	17.623		55.82
ATOM	1365	NH2	ARG	1661	25.394	4.762	19.652		57.53
ATOM	1366	С	ARG	1661	24.139	11.581	14.491	1.00	
ATOM	1367	0	ARG	1661	23.160	12.323	14.401		48.69
ATOM	1368	N	LEU	1662	24.859	11.189	13.440		48.33
ATOM	1369	CA	LEU	1662	24.565	11.647	12.087		45.87
ATOM	1370	CB	LEU	1662	25.839	12.199	11.426		46.18
ATOM	1371	CG	LEU	1662	26.374	13.511	12.016		45.78
ATOM	1372		LEU	1662	27.856	13.681	11.722		45.92
ATOM	1373		LEU	1662	25.576	14.698	11.489		44.92
ATOM	1374	C	LEU	1662	23.961	10.542	11.230		43.02
ATOM	1375	0	LEU	1662	24.647	9.607	10.811		42.04
ATOM	1376	N	PRO	1663	22.648	10.640	10.968		41.48
ATOM	1377	CD	PRO	1663	21.769	11.718	11.468		40.54
ATOM	1378	CA	PRO	1663	21.886	9.680	10.161		39.60
ATOM ATOM	1379	CB	PRO	1663	20.582	10.424	9.889		38.77
ATOM	1380	CG C	PRO	1663 1663	20.386	11.183	11.151		40.83
ATOM	1381 1382		PRO PRO	1663	22.578	9.273	8.860		35.90
ATOM	1382	O N	VAL	1664	22.448 23.356	8.124	8.427 8.276	1.00	36.85
ATOM	1384	CA	VAL	1664	24.053	10.180 9.880	7.024		33.16 32.51
ATOM	1385	CB	VAL	1664	24.851	11.106	6.439		32.31
ATOM	1386		VAL	1664	23.917	12.213	6.065		26.99
ATOM	1387		VAL	1664	25.897	11.607	7.421		29.84
ATOM	1388	C	VAL	1664	24.989	8.675	7.158		30.30
ATOM	1389	0	VAL	1664	25.400	8.091	6.161		30.16
ATOM	1390	N	LYS	1665	25.278	8.276	8.393		27.72
ATOM	1391	CA	LYS	1665	26.170	7.151	8.649		27.96
ATOM	1392	CB	LYS	1665	26.808	7.276	10.025		26.42
ATOM	1393	CG	LYS	1665	27.857	8.351	10.023		28.20
ATOM	1394	CD	LYS	1665	28.221	8.754	11.478		32.47
ATOM	1395	CE	LYS	1665	29.398	9.720	11.468		32.33
ATOM	1396	NZ	LYS	1665	29.713	10.231	12.819		30.38
ATOM	1397	C	LYS	1665	25.522	5.794	8.486		25.81
ATOM	1398	0	LYS	1665	26.159	4.769	8.691		27.53
		•		_000	-9.100	4.700	0.091	1.00	21.55

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		1399	N	TRP	1666	24.	247	5.7	702 0			
		400	CA	TRP	1666		499	4.5		120	1.00	26.13
		401	CB	TRP	1666		259			896	1.00	25.88
		402		TRP	1666	22.		4.5		800	1.00	26.15
TA	_	403	CD2	TRP	1666	23.		4.0		226	1.00	28.12
AT	_	404	CE2	TRP	1666			4.8			1.00	26.14
AT		405	CE3	TRP	1666	23.		4.0			1.00	24.97
ATO	OM 1	406		rrp	1666	23.3		6.2		475	1.00	25.14
TA	_	407		rrp	1666	22.4		2.7	• •	715	1.00	26.09
ATO	DM 14	108		RP	1666	22.7		2.7	51 12.0	34		22.55
ATC		109		RP		23.6		4.45			1.00	25.32
ATC		10	_	'RP	1666	23.7		6.66	4 12.7		1 00	21.72
ATO				'RP	1666	23.9		5.78	12 13.7		1 00	23.77
ATO					1666	23.0		4.44	4 6.4		1 00	23.//
ATO			-	RP	1666	22.6	62	3.39			1.00	24.79
ATO:				ET	1667	23.3	50	5.50			1.00	25.26
ATO			_	ET	1667	22.9		5.56	•		1.00	24.21
ATO	- <del>-</del>			ET	1667	22.7		7.01			1.00	23.79
ATO				ET	1667	21.79		7.81			1.00	25.08
ATO			SD MI		1667	21.77		9.49			1.00	32.58
ATON			CE MI	ET	1667	21.01		9.209			1.00 4	11.43
	_		ME	ET	1667	23.93			_		1.00 4	10.85
ATON			) ME	T	1667	25.13		4.942			.00 2	22.52
ATOM		_	AL	A :	1668	23.40	5	5.173			.00 2	3.63
ATOM		2 ¢	A AL		1668	24.21		4.195		4 1	.00 2	2.77
ATOM		3 C	B AL		1668			3.576		8 1	.00 2	4.91
ATOM		4 C			.668	23.34		2.672		6 1	.00 2	4.41
ATOM		5 0	AL		.668	24.80		4.706		8 1	.00 2	6.66
MOTA	142	6 N	PR		669	24.16		5.748	_	1 1	.00 2	4.54
ATOM	142	7 C			669	26.01		4.511	-0.10	1 1	.00 2	6.97
ATOM	142	8 C2			669	26.93		3.374	0.06	6 1	.00 2	5.23
ATOM	142	9 CI			669	26.614		5.563	-0.91	91.	.00 26	5.05
ATOM	1430			_	669	27.855		4.876	-1.483	2 1.	00 24	1 03
ATOM	1431		PRO			28.259		3.946	-0.358		00 26	. 27
ATOM	1432	_	PRO		669 660	25.687		6.048	-2.030	) 1.	00 26	. 44
ATOM	1433	_	GLU		669	25.576		7.250	-2.263		00 27	
ATOM	1434	-		_	570	24.971		5.137	-2.685		00 27	
ATOM	1435				570	24.093		5.553	-3.769		00 27	. 16
ATOM	1436				570	23.613		1.365	-4.614		00 27	.63
ATOM	1437				70	22.545		.492	-3.980	1.	00 29	. 35
ATOM	1438		GLU		70	23.089		.238	-3.310		00 29	
ATOM		OE			70	22.248		.430	-2.874		00 28	. 03
ATOM	1439		2 GLU	16	70	24.325	2	.040		1.0	00 24	.12
	1440		GLU	16	70	22.931		.407	-3.215	1.0	00 26	. 07
ATOM	1441	0	GLU	16	70	22.477		.281	-3.301	1.0	00 25	. 52
ATOM	1442	N	ALA	16	71	22.452			-4.042	1.0	0 24	12
ATOM	1443	CA	ALA	16	71	21.337		.163	-2.084	1.0	0 27.	74
ATOM	1444	CB	ALA	16				. 928	-1.510	1.0	0 27.	65
ATOM	1445	С	ALA	16		20.729		.189	-0.319	1.0	0 23.	18
ATOM	1446	0	ALA	16		21.860		. 283	-1.065	1.0	0 28.	22
ATOM	1447	N	LEU	16:		21.234		.310	-1.305	1.0	0 28.	51
ATOM	1448	CA	LEU	167		23.011		266	-0.406	1.0	0 30.	60
ATOM	1449	СВ	LEU			23.647		484	0.074	1.0	0 32.	67
ATOM	1450	CG	LEU	167		24.831	9.	127	0.952	1.0	0 32.	0 / 0 E
			النب	167	2	25.662		264	1.527	1.0	0 34.	00
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MOTA	1451	CD1	LEU	1672	24.874	10.981	2.577	1.00 38.85
MOTA	1452	CD2	LEU	1672	26.910	9.667	2.149	1.00 35.22
ATOM	1453	С	LEU	1672	24.121	10.398	-1.067	1.00 37.10
ATOM	1454	0	LEU	1672	23.799	11.580	-1.086	1.00 37.19
MOTA	1455	N	PHE	1673	24.905	9.858	-1.997	1.00 37.60
MOTA	1456	CA	PHE	1673	25.403	10.664	-3.102	1.00 37.11
ATOM	1457	CB	PHE	1673	26.692	10.061	-3.667	1.00 35.24
ATOM	1458	CG	PHE	1673	27.782	9.857	-2.644	1.00 33.54
ATOM	1459	CD1	PHE	1673	28.456	8.633	-2.566	1.00 31.54
MOTA	1460	CD2	PHE	1673	28.143	10.874	-1.762	1.00 33.10
ATOM	1461	CE1	PHE	1673	29.467	8.421	-1.623	1.00 34.66
ATOM	1462	CE2	PHE	1673	29.156	10.678	-0.816	1.00 35.41
ATOM	1463	CZ	PHE	1673	29.819	9.444	-0.748	1.00 34.81
MOTA	1464	C	PHE	1673	24.406	10.890	-4.245	1.00 39.03
MOTA	1465	0	PHE	1673	24.276	11.997	-4.734	1.00 39.02
ATOM	1466	N	ASP	1674	23.693	9.844	-4.651	1.00 42.35
MOTA	1467	CA	ASP	1674	22.757	9.931	-5.762	1.00 41.59
MOTA	1468	CB	ASP	1674	22.957	8.736	-6.700	1.00 46.08
ATOM	1469	CG	ASP	1674	24.384	8.617	-7.201	1.00 51.20
MOTA	1470	OD1	ASP	1674	25.057	9.663	-7.333	1.00 53.97
MOTA	1471	OD2	ASP	1674	24.822	7.470	-7.469	1.00 50.65
MOTA	1472	C	ASP	1674	21.263	9.999	-5.418	1.00 42.89
ATOM	1473	0	ASP	1674	20.427	10.079	-6.317	1.00 41.95
ATOM	1474	N	ARG	1675	20.923	9.899	-4.134	1.00 42.82
ATOM	1475	CA	ARG	1675	19.521	9.944	-3.706	1.00 42.64
ATOM	1476	CB	ARG	1675	18.890	11.300	-4.028	1.00 48.80
ATOM	1477	CG	ARG	1675	19.480	12.449	-3.252	1.00 61.19
ATOM	1478	CD	ARG	1675	19.407	13.727	-4.068	1.00 72.90
ATOM	1479	NE	ARG	1675	20.025	14.854	-3.381	1.00 83.15
MOTA	1480	CZ	ARG	1675	19.652	16.123	-3.539	1.00 88.21
ATOM	1481		ARG	1675	18.662	16.439	-4.365	1.00 89.58
ATOM	1482		ARG	1675	20.265	17.085	-2.860	1.00 92.07
ATOM	1483	C	ARG	1675	18.674	8.825	-4.299	1.00 38.05
MOTA	1484	0	ARG	1675	17.495	9.005	-4.588	1.00 38.87
MOTA	1485	N	ILE	1676	19.281	7.658	-4.479	1.00 34.44
ATOM	1486	CA	ILE	1676	18.576	6.514	-5.012	1.00 30.11
ATOM	1487	CB	ILE	1676	19.378	5.825	-6.096	1.00 29.5B
ATOM	1488	CG2	ILE	1676	18.509	4.850	-6.797	1.00 30.72
ATOM	1489		ILE	1676	19.835	6.868	-7.116	1.00 34.29
ATOM	1490		ILE	1676	20.798	6.348	-8.145	1.00 41.15
ATOM	1491	C	ILE	1676	18.315	5.541	-3.874	1.00 26.90
MOTA	1492	0	ILE	1676	19.236	4.898	-3.364	1.00 22.06
ATOM	1493	N	TYR	1677	17.056	5.465	-3.454	1.00 28.17
ATOM	1494	CA	TYR	1677	16.677	4.589	-2.350	1.00 26.80
MOTA	1495	CB	TYR	1677	15.742	5.310	-1.398	1.00 26.05
ATOM	1496	CG	TYR	1677	16.442	6.367	-0.580	1.00 26.92
ATOM	1497	CD1		1677	16.510	7.693	-1.018	1.00 23.98
ATOM	1498	CE1		1677	17.129	8.665	-0.250	1.00 23.90
ATOM	1499		TYR	1677	17.022	6.048	0.644	1.00 26.99
ATOM	1500		TYR	1677	17.642	7.017	1.414	1.00 24.87
ATOM	1501	CZ	TYR	1677	17.685	8.315	0.968	1.00 26.44
ATOM	1502	OH	TYR	1677	18.227	9.273	1.783	1.00 30.89

ATO	OM 15	03 C	TWD					
ATO		_	TYR TYR		16.		350 -2.	894 1.00 26.30
ATO		_			15.		145 -3.	
ATO			THR		16.4	489 2.1		
ATC			THR	1678	15.9	973 0.9		-100 25.40
ATO			THR	1678	16.9	904 0.3		- 20.27
ATO				1678	18.1			
ATO.				1678	17.0			
ATO		_	THR	1678	15.9	87 -0.0		20.36
ATO		*	THR	1678	16.4			
ATO			HIS	1679	15.5			
ATO	_		HIS	1679	15.4			
ATON			HIS	1679	14.74			
			HIS	1679	13.29			
ATOM			HIS	1679	12.55			
ATOM				1679	12.42			
ATOM				1679	11.20	_		, -, -,
ATOM			HIS	1679	11.25	_		00
ATOM		_	HIS	1679	16.97			00
ATOM			HIS	1679	17.35			5 1.00 20.81
ATOM			GLN	1680	17.79		_	1 1.00 22.50
ATOM	5		GLN	1680	19.24		_	5 1.00 19.58
ATOM	1524	CB		1680	19.86			7 1.00 20.89
ATOM	1525	CG (		1680	19.89			8 1.00 23.76
MOTA	1526	CD (		1680		_		7 1.00 34.08
ATOM	1527	OE1 (		1680	19.019		-	6 1.00 37.77
ATOM	1528	NE2 (		1680	18.069			2 1.00 43.23
MOTA	1529	C G		1680	19.321			3 1.00 37.02
ATOM	1530	0 0	_	1680	19.913			1 1.00 20.72
ATOM	1531			681	20.814	-		1.00 21.53
ATOM	1532			681	19.514		-0.773	1.00 21.01
ATOM	1533			.681	20.128		0.135	1.00 23.86
ATOM	1534			681	19.841		-0.248	1.00 21.10
ATOM	1535			681	18.473		-0.506	1.00 23.18
ATOM	1536			681	19.695		1.564	1.00 23.91
ATOM	1537	N A		682	20.457		2.495	1.00 26.70
ATOM	1538	CA AS		682	18.511	-0.303	1.739	1.00 21.71
ATOM	1539	CB AS		682	18.044	-0.662	3.080	1.00 21.28
ATOM	1540	CG AS		582	16.595	-1.149	3.070	1.00 23.22
ATOM	1541	OD1 AS		582	15.569	-0.016	3.198	1.00 23.08
ATOM	1542	OD2 AS		582 582	14.363	-0.282	3.017	1.00 21.99
ATOM	1543	C AS		582 582	15.948	1.135	3.498	1.00 24.42
ATOM	1544	O AS		82	18.955	-1.756	3.611	1.00 20.86
ATOM	1545	N VA			19.289	-1.770	4.799	1.00 21.62
ATOM	1546	CA VA		83	19.398	-2.649	2.727	1.00 21.60
ATOM		CB VA		83	20.307	-3.732	3.122	1.00 22.27
ATOM		CG1 VA			20.515	-4.740	1.965	1.00 22.22
ATOM		CG2 VA			21.587	-5.777	2.315	1.00 21.52
ATOM		CG2 VAI			19.187	-5.437	1.662	1.00 20.89
ATOM					21.618	-3.150	3.666	1.00 20.89
ATOM					22.107	-3.577	4.705	1.00 21.96
					22.172	-2.160	2.970	1.00 22.01
		CA TRI CB TRI			23.375	-1.489	3.449	1.00 22.01
	-554 (	CB TRE	168	34	23.685	-0.273	2.566	1 00 20 0=
							• •	1.00 20.25

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ATOM	1555	CG	TRP	1684	24.808	0.549	3.069	1.00 22.35
ATOM	1556	CD2		1684	26.118	0.644	2.503	1.00 24.14
ATOM	1557	CE2		1684	26.879	1.500	3.334	1.00 23.68
ATOM	1558	CE3		1684	26.728	0.091	1.370	1.00 25.09
ATOM	1559	CD1		1684	24.825	1.346	4.193	1.00 22.52
ATOM	1560	NE1		1684	26.066	1.915	4.355	1.00 21.48
MOTA	1561	CZ2		1684	28.216	1.815	3.061	1.00 20.56
MOTA	1562	CZ3		1684	28.059	0.405	1.095	1.00 23.92
MOTA	1563	CH2		1684	28.785	1.257	1.942	1.00 23.18
ATOM	1564	С	TRP	1684	23.105	-1.025	4.903	1.00 23.96
MOTA	1565	0	TRP	1684	23.889	-1.308	5.815	1.00 25.98
MOTA	1566	N	SER	1685	21.992	-0.332	5.118	1.00 24.68
MOTA	1567	CA	SER	1685	21.615	0.144	6.447	1.00 22.75
ATOM	1568	CB	SER	1685	20.266	0.870	6.376	1.00 21.11
MOTA	1569	OG	SER	1685	20.276	1.950	5.452	1.00 21.98
ATOM	1570	C	SER	1685	21.516	-1.011	7.457	1.00 23.06
MOTA	1571	0	SER	1685	21.865	-0.850	8.638	1.00 22.55
ATOM	1572	N	PHE	1686	21.041	-2.168	6.998	1.00 21.83
ATOM	1573	CA	PHE	1686	20.915	-3.340	7.854	1.00 21.92
ATOM	1574	CB	PHE	1686	20.153	-4.457	7.129	1.00 18.02
ATOM	1575	CG	PHE	1686	19.965	-5.683	7.971	1.00 20.86
ATOM	1576	CD1	PHE	1686	19.142	-5.641	9.108	1.00 18.76
ATOM	1577	CD2	PHE	1686	20.669	-6.853	7.688	1.00 18.96
MOTA	1578	CE1	PHE	1686	19.023	-6.743	9.947	1.00 19.29
ATOM	1579	CE2	PHE	1686	20.554	-7.965	8.514	1.00 19.27
MOTA	1580	CZ	PHE	1686	19.732	-7.908	9.653	1.00 21.91
ATOM	1581	C	PHE	1686	22.304	-3.845	8.316	1.00 22.11
MOTA	1582	0	PHE	1686	22.473	-4.378	9.436	1.00 21.35
MOTA	1583	N	GLY	1687	23.294	-3.691	7.436	1.00 20.48
MOTA	1584	CA	GLY	1687	24.653	-4.079	7.769	1.00 20.41
ATOM	1585	С	GLY	1687	25.185	-3.211	8.899	1.00 19.03
ATOM	1586	0	GLY	1687	25.857	-3.714	9.808	1.00 20.27
MOTA	1587	N	VAL	1688	24.893	-1.906	8.829	1.00 20.57
MOTA	1588	CA	VAL	1688	25.296	-0.937	9.860	1.00 21.14
MOTA	1589	CB	VAL	1688	24.974	0.548	9.467	1.00 20.78
MOTA	1590	CG1	VAL	1688	25.440	1.493	10.564	1.00 21.51
ATOM	1591	CG2	VAL	1688	25.681	0.923	8.186	1.00 19.70
ATOM	1592	С	VAL	1688	24.547	-1.297	11.142	1.00 23.16
ATOM	1593	0	VAL	1688	25.126	-1.271	12.225	1.00 24.14
MOTA	1594	N	LEU	1689	23.264	-1.648	11.021	1.00 24.50
ATOM	1595	CA	LEU	1689	22.465	-2.058	12.187	1.00 25.93
MOTA	1596	CB	LEU	1689	21.008	-2.316	11.776	1.00 25.42
MOTA	1597	CG	LEU	1689	19.933	-2.392	12.874	1.00 26.29
ATOM	1598	CD1		1689	18.572	-2.053	12.272	1.00 23.43
MOTA	1599	CD2		1689	19.885	-3.768	13.543	1.00 25.66
ATOM	1600	С	LEU	1689	23.080	-3.330	12.797	1.00 28.01
ATOM	1601	0	LEU	1689	23.203	-3.426	14.016	1.00 30.06
ATOM	1602	N	LEU	1690	23.487	-4.287	11.956	1.00 27.19
ATOM	1603	CA	LEU	1690	24.111	-5.520	12.457	1.00 25.29
ATOM	1604	CB	LEU	1690	24.556	-6.446	11.315	1.00 24.98
ATOM	1605	CG	LEU	1690	23.594	-7.390	10.589	1.00 24.85
ATOM	1606	CD1	LEU	1690	24.385	-8.132	9.538	1.00 24.22

	TOM 16	07 CD2	LEU 169	0 22 25
	TOM 16	)8 C	LEU 169	0 -8.434 11.512 1.00 19 10
	TOM 160	9 0	LEU 169	25.326 -5.123 13.291 1.00 24 70
	TOM 161	.0 N	TRP 169	25.521 -5.624 14.408 1 00 27 57
	TOM 161	1 CA	TRP 169:	26.117 -4.197 12.747 1 00 23.57
	POM 161	2 CB	TRP 169	27.316 -3.693 13 425 1 23.00
AI	TOM 161		TRP 1691	27.998 -2.621 12 567
	OM 161		TRP 1691	29.331 -2.173 13 105 3 3-
	'OM 161			29.565 -1.082 14 004 1 22
AT	OM 161		2001	30.966 -0.996 14 208 1 20 23.71
AT	OM 161			28.726 -0.167 14 652 1 00 23.81
AT	OM 1618			30.570 -2.702 12 811 1 20 =
TA				31.550 -1.995 13.471 1.00 24.44
ATO				31.543 -0.000 25.38
ATO			TRP 1691	29.300 0.200 1.00 24.39
ATC			TRP 1691	30,700 0 050
ATO		_	TRP 1691	26,998 3 133
ATO			TRP 1691	27,772 3 322 1.00 25.87
ATO			LU 1692	25.865 2 440 15.750 1.00 27.39
ATO			LU 1692	25,452 -1,060 14.956 1.00 26.45
ATO	0		LU 1692	24.257 -0.000 16.238 1.00 25.13
ATO			LU 1692	24 365 16.068 1.00 23.56
ATO			LU 1692	23 111 0 22 14.962 1.00 18.73
		OE1 G	LU 1692	22 202 0.935 14.880 1.00 23.79
ATON	-050		LU 1692	22 010 0.722 13.962 1.00 22.70
ATOM	_	C G	LU 1692	25 072 1.019 15.738 1.00 25.63
ATOM		O G	LU 1692	25 270 2.363 17.225 1.00 25.28
ATOM		N II	E 1693	2.018 18.422 1 00 27 65
ATOM		CA II		16.720 1.00 26 22
ATOM		CB II		3.164 17.565 1 00 23 03
MOTA		CG2 II		16.787 1.00 22 00
ATOM		CG1 IL	E 1693	7.465 17.637 1.00 21 67
ATOM	1638	CD1 IL		3,369 16 416 3 66
ATOM	1639	C IL		20.964 -6.395 15.435 1 00 13 67
ATOM	1640	O IL		25.322 -5.843 18.133 1 00 24 77
ATOM	1641	N PH		25.401 -6.126 19.324 1.00 34 04
ATOM	1642	CA PHI		26.329 -6.051 17.304 1 00 27 50
ATOM	1643	CB PHE		27.503 -6.709 17.827 1.00 39 42
ATOM	1644	CG PHE		28.122 -7.623 16.771 1 00 30 37
ATOM		CD1 PHE		27.142 -8.649 16 262 7 00 -
ATOM		D2 PHE		26.522 -8.486 15.034 1.00
ATOM		E1 PHE		26.751 -9.709 17 074 7 00 28.43
ATOM		E2 PHE		25.525 -9.355 14.635 1.00 27.86
ATOM		Z PHE		25.751 -10.586 16.674 1.00 30.12
ATOM	1650 C		1694	25.136 -10.408 15 453 7 20
ATOM	1651 0		1694	28.495 -5.821 18.579 1 25
ATOM	1652 N		1694	29.485 -6.305 19.126 1.00 29.83
ATOM			1695	28.217 -4.516 18.635 1.00 32.81
ATOM			1695	29 044 3 500 28.35
ATOM			1695	29 540 2 380
ATOM		THR	1695	28 422 1 622 1.00 21.81
ATOM	1656 CC		1695	30 457 2 225
ATOM	1657 C	THR	1695	28 198 2 126 1.00 16.93
001	1658 O	THR	1695	28 620 2 20.604 1.00 26.16
				28.620 -2.268 21.386 1.00 26.77
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ATOM	1659	N	LEU	1696	27.023	-3.747	20.747	1.00 26.87
ATOM	1660	CA	LEU	1696	26.069	-3.446	21.813	1.00 27.64
MOTA	1661	CB	LEU	1696	26.572	-3.977	23.156	1.00 30.54
ATOM	1662	CG	LEU	1696	26.903	-5.456	23.182	1.00 29.75
ATOM	1663		LEU	1696	27.448	-5.821	24.546	1.00 32.53
ATOM	1664		LEU	1696	25.658	-6.234	22.882	1.00 33.79
ATOM	1665	С	LEU	1696	25.727	-1.984	21.946	1.00 25.51
ATOM	1666	0	LEU	1696	25.824	-1.410	23.025	1.00 27.90
ATOM	1667	N	GLY	1697	25.265	-1.395	20.857	1.00 26.48
ATOM	166B	CA	GLY	1697	24.899	0.007	20.859	1.00 25.81
ATOM	1669	С	GLY	1697	26.040	0.900	20.452	1.00 26.40
ATOM	1670	0	GLY	1697	26.055	2.090	20.760	1.00 29.69
MOTA	1671	N	GLY	1698	27.008	0.330	19.748	1.00 27.65
MOTA	1672	CA	GLY	1698	28.150	1.110	19.314	1.00 28.38
ATOM	1673	C	GLY	1698	27.795	2.186	18.310	1.00 30.13
ATOM	1674	0	GLY	1698	26.896	2.028	17.496	1.00 32.55
ATOM	1675	N	SER	1699	28.520	3.295	18.375	1.00 30.56
ATOM	1676	CA	SER	1699	28.304	4.420	17.491	1.00 32.11
ATOM	1677	CB	SER	1699	28.622	5.714	18.246	1.00 33.58
ATOM	1678	OG	SER	1699	28.578	6.863	17.407	1.00 38.87
ATOM	1679	C	SER	1699	29.203	4.269	16.268	1.00 32.10
ATOM	1680	0	SER	1699	30.408	4.073	16.403	1.00 31.12
ATOM	1681	N	PRO	1700	28.629	4.324	15.062	1.00 32.70
ATOM	1682	CD	PRO	1700	27.204	4.482	14.745	1.00 34.35
MOTA	1683	CA	PRO	1700	29.427	4.192	13.837	1.00 32.25
ATOM	1684	CB	PRO	1700	28.358	4.096	12.736	1.00 32.85
ATOM	1685	CG	PRO	1700	27.101	3.713	13.461	1.00 35.54
ATOM	1686	C	PRO	1700	30.258	5.456	13.651	1.00 31.84
ATOM	1687	0	PRO	1700	29.792	6.550	13.983	1.00 31.56
ATOM	1688	N	TYR	1701	31.487	5.306	13.170	1.00 31.07
ATOM ATOM	1689	CA	TYR	1701	32.372	6.441	12.910	1.00 32.41
MOTA	1690 1691	CB CG	TYR TYR	1701	32.039	7.055	11.537	1.00 32.39
ATOM	1692		TYR	1701 1701	32.088	6.092	10.378	1.00 35.63
ATOM	1693		TYR	1701	30.936	5.807	9.638	1.00 37.94
ATOM	1694		TYR	1701	30.977	4.955	8.535	1.00 40.79
ATOM	1695	CE2	TYR	1701	33.293	5.495	9.990	1.00 37.49
ATOM	1696	CZ	TYR	1701	33.351	4.646 4.382	8.886	1.00 41.82
ATOM	1697	ОН	TYR	1701	32.190 32.251	3.572	8.160	1.00 45.96
ATOM	1698	C	TYR	1701	32.377	7.559	7.039 13.970	1.00 55.61 1.00 32.85
ATOM	1699	ō	TYR	1701	32.066	8.711		1.00 32.85
ATOM	1700	N	PRO	1702	32.753	7.229	13.679 15.215	
ATOM	1701	CD	PRO	1702	33.288	5.946	15.695	1.00 34.48 1.00 35.64
ATOM	1702	CA	PRO	1702	32.775	8.258	16.270	1.00 33.68
ATOM	1703	CB	PRO	1702	33.321	7.499	17.482	
ATOM	1704	CG	PRO	1702	33.063	6.061	17.166	1.00 32.52
ATOM	1705	C	PRO	1702	33.736	9.388		1.00 38.81
ATOM	1706	0	PRO	1702	34.875	9.388	15.919	1.00 33.47
ATOM	1707	N	GLY	1702	33.275	10.625	15.522 16.089	1.00 34.66
ATOM	1708	CA	GLY	1703	34.101	11.792		1.00 35.31 1.00 32.51
ATOM	1709		GLY	1703	34.232	12.166	15.802 14.339	1.00 32.51
ATOM	1710	0	GLY	1703	34.232	13.146	14.339	1.00 33.68
		-			34.504	23.140	74.003	1.00 31.22

ATO		11 N	VAI	1704	77 6				
ATO		12 C			33.5				5.00
ATO		13 C	B VAL		33.6			26 1.00 3	3.25
ATC		14 C	G1 VAL		33.6			41 1.00 3	1.04
ATC			32 VAL		33.8			66 1.00 3:	2.72
ATO	_		VAL	1704	34.8			27 1.00 26	
ATO		7 0	VAL	1704	32.4			33 1.00 34	4.75
ATO	_		PRO	1705	31.3			13 1.00 36	5.79
ATO		9 CD	PRO	1705	32.7 34.1			12 1.00 35	
ATO		0 CA	PRO	1705	31.8			16 1.00 35	6.61
ATO		1 CB	PRO	1705	32.53		_	2 1.00 35	.33
OTA		2 CG	PRO	1705	33.95			7 1.00 35	.59
ATO		3 C	PRO	1705				9 1.00 37	.23
ATON		4 0	PRO	1705	31.38 32.12			4 1.00 36	. 33
ATOM			VAL	1706					. 44
ATOM		CA	VAL	1706	30.24	_		9 1.00 34	. 93
ATOM	_ , _ ,	CB	VAL	1706	29.67			3 1.00 35	.19
ATOM		CG1	VAL	1706	28.60			1.00 36.	.19
AT'OM		CG2	VAL	1706	28.01			1.00 36.	
ATOM	50		VAL	1706	27.49	-		3 1.00 32.	
MOTA		0	VAL	1706	30.69			1.00 36.	20
ATOM		N	GLU	1707	30.796			1.00 38.	16
ATOM	1733	CA	GLU	1707	31.479			1.00 34.	
ATOM	1734	CB	GLU	1707	32.500			1.00 33.	75
ATOM	1735	C	GLU	1707	33.181			1.00 35.	79
ATOM	1736	0	GLU	1707	33.567			1.00 31.	97
ATOM	1737	N		1708	34.036			1.00 32.	
ATOM	1738	CA		1708	33.964			1.00 29.	
ATOM	1739	CB		1708	34.987		6.249	1.00 31.3	32
ATOM	1740	CG		1708	35.567 36.189		7.664	1.00 36.1	
ATOM	1741	CD		1708	37.444	_	8.144	1.00 44.1	
ATOM	1742	OE1	_	1708	38.059	14.923	7.383	1.00 55.5	8
ATOM	1743	OE2	_	1708	37.830	14.082	6.681	1.00 61.4	17
ATOM	1744			708	34.365	16.115	7.517	1.00 60.5	4
ATOM	1745	0		708	35.013	11.906	5.889	1.00 32.2	0
ATOM	1746	N .		.709	33.013	11.041	5.294	1.00 32.3	9
ATOM	1747	CA :		709	32.378	11.749	6.245	1.00 31.4	
ATOM	1748	CB ]		709	30.973	10.522	5.961	1.00 31.7	1
ATOM	1749		LEU 1	709	30.136	10.548	6.565	1.00 28.8	
ATOM	1750	CD1 I	LEU 1	709	30.662	9.357	6.081	1.00 28.28	8
ATOM	1751	CD2 I		709	28.705	8.059	6.679	1.00 27.34	4
ATOM	1752	C I	EU 1	709	32.306	9.556	6.437	1.00 29.71	ı
ATOM	1753	0 1		709	32.489	10.317	4.454	1.00 30.55	5
ATOM	1754	N p		710	32.043	9.202	3.970	1.00 31.79	•
ATOM	1755	CA P		710	31.945	11.399	3.727	1.00 30.99	•
ATOM				710	31.680	11.366	2.279	1.00 32.80	)
ATOM				710	30.310	12.768	1.737	1.00 34.22	:
ATOM	1758	CD1 P		10		13.261	2.020	1.00 37.65	
ATOM	1759	CD2 P		10	29.337	12.393	2.495	1.00 43.43	
ATOM		CE1 P		10	29.984	14.596	1.838	1.00 42.87	
MOTA	1761 (	CE2 PI		10	28.05 <u>4</u> 28.698	12.834	2.787	1.00 46.00	
MOTA			HE 17			15.053	2.130	1.00 46.30	
			-,	_•	27.733	14.169		1.00 46.49	

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ATOM	1763	С	PHE	1710	33.196	10.802	1.667	1.00 34.25
ATOM	1764	0	PHE	1710	33.133	9.948	0.785	1.00 36.09
MOTA	1765	N	LYS	1711	34.324	11.249	2.209	1.00 34.37
MOTA	1766	CA	LYS	1711	35.664	10.840	1.789	1.00 34.11
MOTA	1767	CB	LYS	1711	36.672	11.768	2.476	1.00 37.74
ATOM	1768	CG	LYS	1711	38.114	11.567	2.119	1.00 43.59
MOTA	1769	CD	LYS	1711	38.978	12.573	2.857	1.00 46.97
MOTA	1770	CE	LYS	1711	40.386	12.575	2.304	1.00 51.53
MOTA	1771	NZ	LYS	1711	41.074	11.291	2.603	1.00 58.84
MOTA	1772	C	LYS	1711	35.948	9.354	2.103	1.00 33.25
MOTA	1773	0	LYS	1711	36.512	8.641	1.274	1.00 32.22
MOTA	1774	N	LEU	1712	35.537	8.894	3.285	1.00 32.62
MOTA	1775	CA	LEU	1712	35.718	7.496	3.667	1.00 31.41
MOTA	1776	CB .	LEU	1712	35.223	7.237	5.106	1.00 29.80
MOTA	1777	CG	LEU	1712	36.020	7.889	6.244	1.00 29.22
ATOM	1778	CD1	LEU	1712	35.385	7.643	7.608	1.00 24.09
ATOM	1779	CD2	LEU	1712	37.437	7.356	6.234	1.00 28.36
MOTA	1780	C	LEU	1712	34.939	6.638	2.674	1.00 31.88
MOTA	1781	0	LEU	1712	35.452	5.654	2.143	1.00 34.08
ATOM	1782	N	LEU	1713	33.700	7.029	2.413	1.00 32.28
ATOM	1783	CA	LEU	1713	32.850	6.305	1.482	1.00 35.36
MOTA	1784	CB	LEU	1713	31.433	6.887	1.485	1.00 38.97
MOTA	1785	CG	LEU	1713	30.629	6.494	2.730	1.00 39.56
MOTA	1786		LEU	1713	29.308	7.228	2.768	1.00 37.14
ATOM	1787	CD2	LEU	1713	30.424	4.988	2.748	1.00 37.73
MOTA	1788	С	LEU	1713	33.430	6.296	0.070	1.00 36.47
ATOM	1789	0	LEU	1713	33.502	5.244	-0.563	1.00 39.32
MOTA	1790	N	LYS	1714	33.855	7.455	-0.413	1.00 35.21
ATOM	1791	CA	LYS	1714	34.437	7.544	-1.743	1.00 34.55
ATOM	1792	CB	LYS	1714 .	34.812	8.984	-2.075	1.00 34.81
ATOM	1793	CG	LYS	1714	33.624	9.903	-2.290	1.00 36.55
MOTA	1794	CD	LYS	1714	32.681	9.372	-3.353	1.00 40.68
ATOM	1795	CE	LYS	1714	31.488	10.310	-3.577	1.00 44.87
ATOM	1796	NZ	LYS	1714	30.611	9.853	-4.701	1.00 50.99
ATOM	1797	C	LYS	1714	35.671	6.649	-1.856	1.00 35.97
ATOM	1798	0	LYS	1714	35.948	6.084	-2.920	1.00 38.11
ATOM	1799	N	GLU	1715	36.385	6.490	-0.749	1.00 33.65
MOTA	1800	CA	GLU	1715	37.582	5.663	-0.729	1.00 34.34
MOTA	1801	CB	GLU	1715	38.574	6.221	0.288	1.00 34.90
MOTA	1802	CG	GLU	1715	39.032	7.613	-0.110	1.00 42.07
ATOM	1803	CD	GLU	1715	39.729	8.405	0.989	1.00 47.94
ATOM	1804	OE1		1715	39.977	7.870	2.098	1.00 45.03
ATOM	1805	OE2		1715	40.026	9.596	0.709	1.00 51.48
MOTA	1806	C	GLU	1715	37.285	4.191	-0.466	1.00 34.76
ATOM	1807	0	GLU	1715	38.205	3.384	-0.411	1.00 37.36
ATOM	1808	N	GLY	1716	36.002	3.848	-0.347	1.00 32.00
ATOM	1809	CA	GLY	1716	35.604	2.474	-0.122	1.00 30.49
ATOM	1810	C	GLY	1716	35.932	1.937	1.251	1.00 31.32
ATOM	1811	0	GLY	1716	36.134	0.738	1.430	1.00 31.83
ATOM	1812	N	HIS	1717	35.957	2.822	2.233	1.00 31.55
ATOM	1813	CA	HIS	1717	36.265	2.416	3.595	1.00 33.20
MOTA	1814	CB	HIS	1717	36.494	3.661	4.452	1.00 37.67

AT	OM 1815	CG HIS 1717	
AT	OM 1816	1110 1/1/	3,360 5,895 1 00 45 45
	OM 1817	1717	37 957 3 350
	OM 1818	071	35 789 3 149
AT		171/	36.333 2 034
AT		NE2 HIS 1717	37.645 2.076
AT		C HIS 1717	35.149 1 567
ATO		O HIS 1717	33.975 1.026 1.201 1.00 31.72
ATO		N ARG 1718	35 529 0 500
		CA ARG 1718	34 586 0 300
ATC		CB ARG 1718	34 521
ATC		CG ARG 1718	34 040 5.024 1.00 31.61
ATO		CD ARG 1718	32.570 3.577 1.00 31.32
ATO	,	NE ARG 1718	3.495 1.00 29 60
ATO	M 1828	CZ ARG 1718	2.129 1 00 24 22
ATO		NH1 ARG 1718	32.103 -0.324 1.243 1.00 22 01
ATO	M 1830	NH2 ARG 1718	32.709 0.819 1.554 1 00 19 00
ATO		C ARG 1718	0.083 1.00 14.10
ATO	M 1832	2.5 1,18	35.042 -0.438 7.164 1.00 32.01
ATO		1716	36.234 -0.596 7.446 1.00 34.50
ATON	1 1834	7	34.084 -0.372 8.085 1.00 22 05
ATOM	1 1835	2713	34.382 -0.466 9.508 1.00 33.99
ATOM		1/19	33.110 ~0.246 10 342 1 00 00
ATOM		2713	32 512 3 355
ATOM		SD MET 1719 CE MET 1719	31 002 1 506
ATOM		113	29 906 0 37.49
ATOM	***	C MET 1719	35 032 1 700
ATOM		O MET 1719	34,900 -2 772
ATOM	-0.1	N ASP 1720	35 776 7 005
ATOM		CA ASP 1720	36 466 3 030
ATOM		CB ASP 1720	37 585 2 501 1.00 36.87
ATOM		G ASP 1720	38 688 3 550 1.00 41.64
ATOM		DD1 ASP 1720	38 507 7 430
		D2 ASP 1720	39 740 7 550
ATOM	1847 C	ASP 1720	35 516 4 505 12.422 1.00 46.76
ATOM	1848 O	ASP 1720	34 459 3 500 12.053 1.00 34.70
MOTA	1849 N	LYS 1721	35 022 12.548 1.00 34.31
ATOM	1850 C		35 110 33.265 12.132 1.00 33.39
ATOM	1851 C		35 600 - 12.755 1.00 32.68
ATOM	1852 C	· · · ·	34 034 17.690 12.500 1.00 33.55
ATOM	1853 CI		25 22 2 2 3 2 3 2 3 2 3 2 3 2 3 2 3 2 3
ATOM	1854 CE		12.771 1.00 35 77
ATOM	1855 N2	_ · · · ·	30.082 -10.747 13 931 1 00 75
ATOM	1856 C	LYS 1721	33.323 -12.190 13.711 1 00 43 86
ATOM	1857 O	LYS 1721	35.034 -6.107 14.240 1.00 34.61
ATOM	1858 N		14.905 1.00 37 05
ATOM	1859 CD		33.808 -6.092 14.781 1 00 36
ATOM	1860 CA		32.518 -6.062 14.066 1 00 34 75
ATOM	1861 CB	2,22	33.611 -5.926 16.222 1 00 27 2
ATOM			32.095 -6.017 16.360 1.00 37.84
ATOM			31 607 5 445
ATOM	1863 C 1864 O	PRO 1722	34 266 7 200
ATOM		PRO 1722	34 340 0 000
ATOM	1865 N	SER 1723	34 783 6 224
014	1866 CA	SER 1723	35 359 7 007 1.00 42.36
			35.359 -7.995 18.890 1.00 45.70

MOTA	1867	CB	SER	1723	36.170	-7.511	20.093	1.00 47.50
MOTA	1868	OG	SER	1723	35.341	-6.964	21.100	1.00 55.28
MOTA	1869	С	SER	1723	34.136	-8.784	19.346	1.00 46.70
ATOM	1870	0	SER	1723	33.037	-8.224	19.477	1.00 47.27
ATOM	1871	N	ASN	1724	34.296	-10.081	19.559	1.00 47.84
ATOM	1872	CA	ASN	1724	33.174	-10.900	19.992	1.00 51.26
MOTA	1873	CB	ASN	1724	32.620	-10.361	21.330	1.00 57.15
MOTA	1874	CG	ASN	1724	33.732	-10.088	22.365	1.00 61.53
ATOM	1875	OD1	ASN	1724	34.565	-10.955	22.646	1.00 64.13
MOTA	1876	ND2	ASN	1724	33.763	-8.867	22.912	1.00 61.69
MOTA	1877	С	ASN	1724	32.101	-10.916	18.873	1.00 50.72
ATOM	1878	0	ASN	1724	30.925	-10.617	19.089	1.00 52.63
ATOM	1879	N	CYS	1725	32.564	-11.193	17.663	1.00 48.01
MOTA	1880	CA	CYS	1725	31.719	-11.295	16.478	1.00 45.16
MOTA	1881	CB	CYS	1725	31.603	-9.929	15.788	1.00 44.77
ATOM	1882	SG	CYS	1725	30.605	-9.929	14.272	1.00 40.74
ATOM	1883	C	CYS	1725	32.421	-12.308	15.570	1.00 41.51
ATOM	1884	0	CYS	1725	33.639	-12.236	15.397	1.00 42.47
MOTA	1885	N	THR	1726	31.677	-13.289	15.064	1.00 37.54
MOTA	1886	CA	THR	1726	32.268	-14.313	14.202	1.00 35.03
ATOM	1887	CB	THR	1726	31.308	-15.500	13.993	1.00 31.87
ATOM	1888	OG1	THR	1726	30.074	-15.042	13.406	1.00 32.84
ATOM	1889	CG2	THR	1726	31.017	-16.160	15.306	1.00 29.78
ATOM	1890	С	THR	1726	32.678	-13.770	12.845	1.00 34.76
MOTA	1891	0	THR	1726	32.180	-12.729	12.415	1.00 38.22
MOTA	1892	N	ASN	1727	33.596	-14.450	12.175	1.00 32.47
ATOM	1893	CA	ASN	1727	34.009	-14.024	10.842	1.00 34.75
ATOM	1894	CB	ASN	1727	35.167	-14.872	10.308	1.00 39.77
ATOM	1895	CG	ASN	1727	36.464	-14.591	11.026	1.00 46.09
MOTA	1896		ASN	1727	37.019	-13.495	10.933	1.00 49.54
ATOM .	1897		ASN	1727	36.961	-15.585	11.749	1.00 50.04
MOTA	1898	С	ASN	1727		-14.147	9.905	1.00 33.38
ATOM	1899	0	ASN	1727		-13.405	8.929	1.00 34.10
ATOM	1900	N	GLU	1728		-15.065	10.224	1.00 32.01
ATOM	1901	CA	GLU	1728	30.707	-15.310	9.418	1.00 30.41
ATOM	1902	CB	GLU	1728		-16.580	9.917	1.00 32.27
MOTA	1903	CG	GLU	1728		-17.034	9.094	1.00 31.55
ATOM	1904	CD	GLU	1728		-18.369	9.577	1.00 36.38
MOTA	1905	OE1	GLU	1728		-18.694	10.777	1.00 38.35
ATOM	1906		GLU	1728		-19.086	8.758	1.00 36.34
ATOM	1907	С	GLU	1728		-14.119	9.468	1.00 29.40
ATOM	1908	0	GLU	1728		-13.679	8.438	1.00 26.23
MOTA	1909	N	LEU	1729		-13.610	10.672	1.00 29.19
ATOM	1910	CA	LEU	1729		-12.462	10.849	1.00 30.26
MOTA	1911	CB	LEU	1729		-12.343	12.310	1.00 30.74
ATOM	1912	CG	LEU	1729		-13.410	12.721	1.00 31.27
ATOM	1913		LEU	1729		-13.377	14.226	1.00 33.65
ATOM	1914	CD2		1729		-13.161	12.010	1.00 26.16
ATOM	1915	С	LEU	1729		-11.161	10.335	1.00 28.79
ATOM	1916	0	LEU	1729			9.914	1.00 30.60
ATOM	1917	N	TYR	1730		-11.069	10.363	1.00 26.64
ATOM	1918	CA	TYR	1730	31.281	-9.881	9.844	1.00 26.47



ATOM 1919 CB TYR 1730 32.742 -9.869 10.298 1.00 24.31 ATOM 1921 CD1 TYR 1730 33.512 -8.670 9.805 1.00 25.61 ATOM 1922 CC1 TYR 1730 33.512 -8.670 9.805 1.00 25.61 ATOM 1923 CC2 TYR 1730 33.691 -6.264 9.496 1.00 23.70 ATOM 1924 CE2 TYR 1730 33.691 -6.264 9.496 1.00 23.70 ATOM 1925 CZ TYR 1730 34.688 -8.826 9.667 1.00 24.37 ATOM 1925 CZ TYR 1730 34.688 -8.826 9.667 1.00 24.37 ATOM 1925 C TYR 1730 34.856 -6.445 8.746 1.00 24.37 ATOM 1926 ON TYR 1730 30.981 -9.902 8.301 1.00 26.60 ATOM 1927 C TYR 1730 30.981 -9.902 8.301 1.00 26.60 ATOM 1928 O TYR 1731 31.347 -11.084 7.727 1.00 26.60 ATOM 1931 CR MET 1731 31.347 -11.270 5.996 1.00 29.90 ATOM 1931 CR MET 1731 31.475 -12.740 5.966 1.00 38.39 ATOM 1932 CG MET 1731 31.076 -13.157 4.577 1.00 25.98 ATOM 1933 C MET 1731 32.659 -14.506 2.727 1.00 66.05 ATOM 1938 C MET 1731 29.864 -10.819 4.791 1.00 20.69.79 ATOM 1938 C MET 1731 29.864 -10.819 5.840 1.00 29.05 ATOM 1939 C MET 1732 29.864 -10.819 5.840 1.00 29.05 ATOM 1939 C MET 1732 29.864 -10.819 5.840 1.00 29.05 ATOM 1939 C MET 1732 29.864 -10.819 5.840 1.00 29.05 ATOM 1939 C MET 1732 29.864 -10.819 5.840 1.00 29.05 ATOM 1939 C MET 1732 29.864 -10.819 5.840 1.00 29.05 ATOM 1939 C MET 1732 29.864 -10.819 5.840 1.00 29.05 ATOM 1940 CG MET 1732 27.475 -10.743 6.633 1.00 29.05 ATOM 1940 CG MET 1732 27.475 -10.743 6.633 1.00 29.05 ATOM 1941 SD MET 1732 27.475 -10.743 6.633 1.00 29.07 ATOM 1942 C MET 1732 28.845 11.134 6.633 1.00 29.07 ATOM 1943 C MET 1732 29.864 -10.819 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.929 7.92	_				
ATOM 1920 CG TYR 1730 33.512 -8.670 9.805 10.00 24.31 ATOM 1921 CD1 TYR 1730 33.0529 -7.373 10.016 1.00 25.68 ATOM 1923 CD2 TYR 1730 33.0591 -6.264 9.496 1.00 23.70 24.41 ATOM 1925 CZ TYR 1730 34.688 -8.626 9.697 1.00 24.48 ATOM 1926 CD TYR 1730 34.688 -8.626 9.697 1.00 24.48 ATOM 1926 CD TYR 1730 34.688 -8.626 9.697 1.00 24.48 ATOM 1926 CD TYR 1730 34.686 -9.902 8.301 1.00 24.41 ATOM 1928 CD TYR 1730 34.686 -9.902 8.301 1.00 24.41 ATOM 1928 CD TYR 1730 34.856 -6.445 8.467 1.00 24.41 ATOM 1928 CD TYR 1730 34.856 -6.455 8.467 1.00 24.41 ATOM 1928 CD TYR 1730 34.856 -9.902 8.301 1.00 26.06 ATOM 1929 N MET 1731 31.186 -9.902 8.301 1.00 26.06 ATOM 1929 N MET 1731 31.247 -11.270 6.299 1.00 29.90 ATOM 1931 CG MET 1731 31.475 -12.740 5.968 1.00 24.37 ATOM 1931 CE MET 1731 31.475 -12.740 5.968 1.00 29.90 ATOM 1933 CD MET 1731 31.612 -14.831 4.266 1.00 69.59 ATOM 1935 CD MET 1731 31.612 -14.831 4.266 1.00 69.59 ATOM 1936 CD MET 1731 32.659 -14.506 2.727 1.00 66.05 ATOM 1937 N MET 1732 29.864 -10.894 7.797 1.00 66.05 ATOM 1938 CD MET 1732 29.864 -10.894 7.798 1.00 29.90 ATOM 1938 CD MET 1732 29.864 -10.894 7.798 1.00 29.90 ATOM 1938 CD MET 1732 29.864 -10.894 7.798 1.00 29.90 ATOM 1938 CD MET 1732 27.475 -10.743 6.228 1.00 29.90 ATOM 1944 CD MET 1732 27.475 -10.743 6.228 1.00 29.90 ATOM 1940 CG MET 1732 27.475 -10.743 6.228 1.00 29.90 ATOM 1940 CG MET 1732 27.475 -10.743 6.228 1.00 29.90 ATOM 1941 CD MET 1732 27.475 -10.984 7.156 1.00 29.573 ATOM 1940 CG MET 1732 27.475 -10.984 7.156 1.00 29.573 ATOM 1940 CG MET 1732 27.475 -10.984 7.156 1.00 29.573 ATOM 1940 CG MET 1733 28.695 -14.506 2.797 1.00 24.99 ATOM 1940 CG MET 1732 27.475 -10.984 7.156 1.00 29.79 ATOM 1940 CG MET 1732 27.475 -10.984 7.156 1.00 29.573 ATOM 1940 CG MET 1732 27.475 -10.984 7.156 1.00 29.573 ATOM 1940 CG MET 1733 28.695 -10.984 7.156 1.00 29.59 ATOM 1940 CG MET 1733 28.695 -10.984 7.156 1.00 29.59 ATOM 1940 CG MET 1733 28.695 -10.984 7.156 1.00 29.59 ATOM 1940 CG MET 1733 28.695 -10.985 7.156 1.00 29.59 ATOM 1940 CG MET 1733 28.695 -10.984 7.156 1.0			9 CB	TYR 17	30 - 20 -
ATOM 1921 CD1 TYR 1730 33.029 -7.373 10.016 1.00 25.61 ATOM 1923 CD2 TYR 1730 33.691 -6.264 9.496 1.00 23.70 ATOM 1924 CD2 TYR 1730 33.691 -6.264 9.496 1.00 23.70 ATOM 1925 CZ TYR 1730 33.691 -6.264 9.496 1.00 24.41 ATOM 1926 CD TYR 1730 34.688 -8.826 9.067 1.00 24.41 ATOM 1926 CD TYR 1730 35.361 -7.719 8.537 1.00 24.41 ATOM 1926 CD TYR 1730 35.466 -5.454 8.748 1.00 24.41 ATOM 1928 O TYR 1730 35.466 -5.554 8.166 1.00 24.41 ATOM 1928 O TYR 1730 35.476 -5.554 8.167 1.00 23.68 ATOM 1928 O TYR 1730 35.476 -5.554 8.176 1.00 23.68 ATOM 1929 N MET 1731 31.186 -9.902 8.301 1.00 24.37 ATOM 1928 O TYR 1730 31.186 -9.902 8.301 1.00 24.37 ATOM 1931 CB MET 1731 31.247 -11.270 6.299 1.00 29.90 ATOM 1931 CB MET 1731 31.475 -11.270 6.299 1.00 29.90 ATOM 1931 CB MET 1731 31.076 -13.157 4.577 1.00 38.39 ATOM 1933 SD MET 1731 31.076 -13.157 4.577 1.00 52.98 ATOM 1934 C MET 1731 32.659 -14.506 2.727 1.00 66.05 ATOM 1938 CA MET 1731 22.659 -14.506 2.727 1.00 66.05 ATOM 1938 CA MET 1731 22.720 -10.194 4.791 1.00 29.05 ATOM 1939 CB MET 1732 28.845 -11.134 6.633 1.00 29.40 ATOM 1930 CB MET 1732 28.845 -11.134 6.633 1.00 29.40 ATOM 1930 CB MET 1732 27.475 -10.194 4.791 1.00 29.05 ATOM 1941 SD MET 1732 27.475 -10.194 4.791 1.00 29.05 ATOM 1941 SD MET 1732 27.475 -10.194 4.791 1.00 20.95 ATOM 1941 SD MET 1732 27.475 -10.194 4.791 1.00 20.95 ATOM 1943 C MET 1732 27.475 -10.194 4.791 1.00 20.95 ATOM 1944 O MET 1732 27.475 -10.194 4.791 1.00 20.95 ATOM 1944 O MET 1732 27.387 -9.220 6.271 1.00 27.79 ATOM 1944 O MET 1732 27.387 -9.220 6.271 1.00 27.79 ATOM 1944 O MET 1733 28.00 -11.637 8.407 1.00 29.55 ATOM 1945 C MET 1733 28.00 -11.637 8.407 1.00 29.55 ATOM 1945 C MET 1733 28.00 -11.637 8.407 1.00 29.55 ATOM 1945 C MET 1733 28.00 -11.637 8.407 1.00 29.55 ATOM 1945 C MET 1733 28.80 -7.423 1.127 1.00 21.23 ATOM 1946 C MET 1733 28.80 -7.423 1.127 1.00 21.23 ATOM 1946 C MET 1733 28.80 -7.423 1.127 1.00 21.23 ATOM 1955 C MET 1733 28.80 -7.423 1.127 1.00 21.23 ATOM 1955 C MET 1733 28.80 -7.423 1.127 1.00 21.23 ATOM 1955 C MET 1733 28.80 -7.423 1.1			0 CG		30 -9.869 10.298 1 00 34 34
ATOM 1922 CEI TYR 1730 33.099 -7.373 10.016 1.00 25.68 ATOM 1923 CDZ TYR 1730 33.691 -6.264 9.496 1.00 23.70 ATOM 1925 CEZ TYR 1730 34.688 -8.26 9.607 1.00 23.70 ATOM 1926 CEZ TYR 1730 34.688 -8.26 9.607 1.00 23.70 ATOM 1926 CEZ TYR 1730 34.686 -6.264 9.496 1.00 23.70 ATOM 1927 CEZ TYR 1730 34.686 -6.455 8.748 1.00 24.41 ATOM 1928 OF TYR 1730 34.686 -6.455 8.748 1.00 24.41 ATOM 1928 OF TYR 1730 34.686 -6.455 8.748 1.00 24.41 ATOM 1928 OF TYR 1730 34.866 -6.455 8.748 1.00 24.41 ATOM 1928 OF TYR 1730 34.868 -8.26 9.902 8.301 1.00 26.06 ATOM 1928 OF TYR 1730 34.866 -6.455 8.8176 1.00 24.41 ATOM 1928 OF TYR 1730 34.866 -6.455 8.8176 1.00 24.41 ATOM 1928 OF TYR 1730 34.866 -6.455 8.8176 1.00 24.43 ATOM 1928 OF TYR 1731 34.186 -9.902 8.301 1.00 26.06 ATOM 1928 OF TYR 1731 34.186 -9.902 8.301 1.00 26.06 ATOM 1931 CE MET 1731 34.47 -11.270 6.299 1.00 29.90 ATOM 1933 CM MET 1731 34.475 -12.740 5.968 1.00 38.39 ATOM 1933 CM MET 1731 34.665 -14.506 2.727 1.00 66.05 ATOM 1933 CM MET 1731 34.665 -14.506 2.727 1.00 66.05 ATOM 1933 CM MET 1731 29.864 -10.819 5.840 1.00 29.05 ATOM 1936 CM MET 1731 29.864 -10.819 5.840 1.00 29.05 ATOM 1938 CM MET 1732 28.865 -11.134 6.633 1.00 29.40 ATOM 1938 CM MET 1732 28.659 -14.506 6.331 1.00 29.40 ATOM 1934 CM MET 1732 27.475 -10.743 6.328 1.00 26.97 ATOM 1941 SD MET 1732 27.475 -10.743 6.328 1.00 26.97 ATOM 1941 SD MET 1732 27.475 -10.743 6.328 1.00 26.97 ATOM 1944 CM MET 1732 27.387 -9.220 6.271 1.00 26.05 ATOM 1945 N MET 1732 27.387 -9.220 6.271 1.00 27.49 ATOM 1945 N MET 1733 28.001 -7.090 7.293 1.00 27.49 ATOM 1945 N MET 1733 28.001 -7.090 7.293 1.00 27.49 ATOM 1940 CM MET 1733 28.001 -7.090 7.293 1.00 27.49 ATOM 1940 CM MET 1733 28.001 -7.090 7.293 1.00 27.49 ATOM 1940 CM MET 1733 28.001 -7.090 7.293 1.00 27.49 ATOM 1950 CM MET 1733 28.001 -7.090 7.293 1.00 27.49 ATOM 1955 CM ARG 1734 38.855 -5.288 4.499 1.00 38.74 ATOM 1955 CM ARG 1734 38.855 -5.288 4.499 1.00 38.74 ATOM 1955 CM ARG 1734 38.669 -7.669 4.551 1.00 26.58 ATOM 1955 CM ARG 1734 33.855 -5.288 4.499 1.00 27.27 ATOM 1956 CM	A	TOM 192	1 CD1		33.512 -8.670 9 806 1 22.31
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ATOM 1951 C MET 1733 28.850 -7.423 12.399 1.00 33.03 28.711 -6.599 6.035 1.00 28.54 28.711 -6.599 6.035 1.00 28.54 28.711 -6.599 6.035 1.00 28.54 28.711 -6.599 6.035 1.00 28.54 28.711 29.865 29.865 27.194 5.751 1.00 30.69 28.59 29.865 27.194 5.751 1.00 28.59 29.865 27.194 29.865 27.194 5.751 1.00 28.59 29.860 29.860 29.865 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860 29.860		1950		55	29.300 -6.248 11.127 1 00 22 75
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ATOM 1954 CA ARG 1734 ATOM 1955 CB ARG 1734 ATOM 1956 CG ARG 1734 ATOM 1957 CD ARG 1734 ATOM 1958 NE ARG 1734 ATOM 1959 CZ ARG 1734 ATOM 1960 NH1 ARG 1734 ATOM 1961 NH2 ARG 1734 ATOM 1962 C ARG 1734 ATOM 1963 O ARG 1734 ATOM 1964 N ASP 1735 ATOM 1966 CB ASP 1735 ATOM 1968 OD1 ASP 1735 ATOM 1969 OD2 ASP 1735		1953 I	_		28.250 -5.680 5.357 7.00
ATOM 1955 CB ARG 1734 31.970 -7.609 4.531 1.00 29.53 ATOM 1956 CG ARG 1734 32.944 -7.245 5.638 1.00 26.75 ATOM 1958 NE ARG 1734 33.158 -5.755 5.702 1.00 26.58 ATOM 1959 CZ ARG 1734 33.825 -5.288 4.499 1.00 34.72 ATOM 1960 NH1 ARG 1734 35.139 -5.360 4.306 1.00 37.67 ATOM 1961 NH2 ARG 1734 35.927 -5.867 5.251 1.00 40.46 ATOM 1962 C ARG 1734 35.663 -4.986 3.147 1.00 38.11 ATOM 1963 O ARG 1734 29.855 -7.051 3.294 1.00 28.03 ATOM 1964 N ASP 1735 29.071 -8.130 3.260 1.00 27.22 ATOM 1966 CB ASP 1735 29.071 -8.130 3.260 1.00 27.27 ATOM 1967 CG ASP 1735 28.212 -8.436 2.103 1.00 27.27 ATOM 1968 OD1 ASP 1735 28.638 -10.932 2.075 1.00 30.15 ATOM 1969 OD2 ASP 1735 28.354 -12.070 2.501 1.00 32.00 ATOM 1970 C ASP 1735 27.099 -7.400 1.971 1.00 24.78	ATOM	100.		• •	29.865 -7.194 5 751 3 00 30.69
ATOM 1956 CG ARG 1734 ATOM 1957 CD ARG 1734 ATOM 1958 NE ARG 1734 ATOM 1959 CZ ARG 1734 ATOM 1959 CZ ARG 1734 ATOM 1960 NH1 ARG 1734 ATOM 1961 NH2 ARG 1734 ATOM 1962 C ARG 1734 ATOM 1963 O ARG 1734 ATOM 1964 N ASP 1735 ATOM 1966 CB ASP 1735 ATOM 1968 OD1 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1970 C ASP 1735	ATOM	300-			30.650 -6.831 4.571 1.00 28.59
ATOM 1957 CD ARG 1734 ATOM 1958 NE ARG 1734 ATOM 1959 CZ ARG 1734 ATOM 1960 NH1 ARG 1734 ATOM 1961 NH2 ARG 1734 ATOM 1962 C ARG 1734 ATOM 1963 O ARG 1734 ATOM 1964 N ASP 1735 ATOM 1966 CB ASP 1735 ATOM 1968 OD1 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1970 C ASP 1735	ATOM				31.970 -2.600
ATOM 1958 NE ARG 1734 ATOM 1959 CZ ARG 1734 ATOM 1960 NH1 ARG 1734 ATOM 1961 NH2 ARG 1734 ATOM 1962 C ARG 1734 ATOM 1963 O ARG 1734 ATOM 1964 N ASP 1735 ATOM 1966 CB ASP 1735 ATOM 1967 CG ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1970 C ASP 1735	ATOM				32.944 7 245
ATOM 1959 CZ ARG 1734 ATOM 1960 NH1 ARG 1734 ATOM 1961 NH2 ARG 1734 ATOM 1962 C ARG 1734 ATOM 1963 O ARG 1734 ATOM 1964 N ASP 1735 ATOM 1966 CB ASP 1735 ATOM 1968 OD1 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1969 CC ASP 1735 ATOM 1969 OD2 ASP 1735 ATOM 1970 C ASP 1735					33.158 = 5.755 1.00 26.75
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ATOM 1966 CB ASP 1735 27.608 -9.835 2.216 1.00 27.27 ATOM 1968 OD1 ASP 1735 28.638 -10.932 2.075 1.00 30.15 ATOM 1969 OD2 ASP 1735 29.745 -10.663 1.553 1.00 31.23 ATOM 1970 C ASP 1735 27.099 -7.400 1.971 1.00 24.78			ASP		3,260 1 00 27 07
ATOM 1967 CG ASP 1735 28.638 -10.932 2.075 1.00 30.15 ATOM 1969 OD2 ASP 1735 29.745 -10.663 1.553 1.00 31.23 ATOM 1970 C ASP 1735 28.354 -12.070 2.501 1.00 32.00 27.099 -7.400 1.971 1.00 24.78		1966 CE			28.212 -8.436 2.103 1 00 27 27
ATOM 1968 OD1 ASP 1735 28.638 -10.932 2.075 1.00 28.62 ATOM 1969 OD2 ASP 1735 29.745 -10.663 1.553 1.00 31.23 ATOM 1970 C ASP 1735 28.354 -12.070 2.501 1.00 32.00 27.099 -7.400 1.971 1.00 24.78					27.608 -9.835 2 216 3 2
ATOM 1969 OD2 ASP 1735 29.745 -10.663 1.553 1.00 31.23 ATOM 1970 C ASP 1735 28.354 -12.070 2.501 1.00 32.00 27.099 -7.400 1.971 1.00 24.78					28.638 -10.932 2.075 1.00 30 3-
ATOM 1970 C ASP 1735 28.354 -12.070 2.501 1.00 32.00 27.099 -7.400 1.971 1.00 24.78			2 ASD		29.745 -10.663 1 553
27.099 -7.400 1.971 1.00 24.78	ATOM				28.354 -12.070 2 501 7 7
1.9/1 1.00 24.78		_	ASP	1/35	27.099 7.400
					1.00 24.78

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ATOM	1971	0	ASP	1735	26.714	-7.068	0.852	1.00	24.52
ATOM	1972	N	CYS	1736	26.590	-6.908	3.104	1.00	24.10
ATOM	1973	CA	CYS	1736	25.530	-5.871	3.140		25.20
ATOM	1974	CB	CYS	1736	24.965	-5.679	4.569		23.85
MOTA	1975	SG	CYS	1736	23.898	-7.030	5.143		
ATOM	1976	С	CYS	1736	26.042	-4.520	2.611		23.39
ATOM	1977	0	CYS	1736	25.276	-3.718	2.070		21.76
ATOM	1978	N	TRP	1737	27.348	-4.303	2.743		23.53
ATOM	1979	CA	TRP	1737	27.988	-3.072	2.302		21.57
ATOM	1980	СВ	TRP	1737	29.026	-2.631	3.314		18.82
ATOM	1981	CG	TRP	1737	28.485	-2.418	4.686		19.89
ATOM	1982	CD2	TRP	1737	29.194	-2.609	5.913		22.39
ATOM	1983	CE2		1737	28.329	-2.213	6.959		21.78
ATOM	1984		TRP	1737	30.478	-3.083	6.238		23.52
ATOM	1985		TRP	1737	27.248	-1.932	5.022		19.40
ATOM	1986		TRP	1737	27.147	-1.805	6.383		21.52
ATOM	1987	CZ2	TRP	1737	28.705	-2.270	8.319		21.85
ATOM	1988	CZ3	TRP	1737	30.857	-3.134	7.583		25.30
ATOM	1989	CH2	TRP	1737	29.972	-2.728	8.604		26.17
ATOM	1990	С	TRP	1737	28.673	-3.226	0.956		24.49
ATOM	1991	О	TRP	1737	29.648	-2.519	0.670		25.09
ATOM	1992	N	HIS	1738	28.203	-4.170	0.136	1.00	
ATOM	1993	CA	HIS	1738	28.808	-4.341	-1.172		22.90
ATOM	1994	СВ	HIS	1738	28.163	-5.497	-1.928		23.14
ATOM	1995	CG	HIS	1738	29.017	-6.013	-3.051	1.00	
ATOM	1996	CD2	HIS	1738	29.550	-5.380	-4.129	1.00	
ATOM	1997		HIS	1738	29.492	-7.308	-3.104	1.00	
ATOM	1998	CE1	HIS	1738	30.286	-7.445	-4.156	1.00	
ATOM	1999	NE2	HIS	1738	30.341	-6.288	-4.794	1.00	
ATOM	2000	С	HIS	1738	28.670	-3.024	-1.958	1.00	
MOTA	2001	0	HIS	1738	27.615	-2.381	-1.933	1.00	
ATOM	2002	N	ALA	1739	29.752	-2.608	-2.607	1.00	
MOTA	2003	CA	ALA	1739	29.762	-1.378	-3.385	1.00	23.70
ATOM	2004	СВ	ALA	1739	31.079	-1.234	-4.076	1.00	25.24
MOTA	2005	С	ALA	1739	28.645	-1.391	-4.416	1.00	25.37
MOTA	2006	0	ALA	1739	27.955	-0.391	-4.606	1.00	27.86
MOTA	2007	N	VAL	1740	28.507	-2.521	-5.102	1.00	23.97
MOTA	2008	CA	VAL	1740	27.481	-2.700	-6.121	1.00	24.64
ATOM	2009	CB	VAL	1740	27.966	-3.698	-7.206	1.00	26.39
MOTA	2010	CG1	VAL	1740	27.013	-3.757	-8.360	1.00	22.65
ATOM	2011	CG2	VAL	1740	29.308	-3.260	-7.720	1.00	27.43
ATOM	2012	С	VAL	1740	26.170	-3.209	-5.481	1.00	23.97
ATOM	2013	0	VAL	1740	26.126	-4.347	-4.978	1.00	24.14
MOTA	2014	N	PRO	1741	25.090	-2.397	-5.545	1.00	22.77
MOTA	2015	CD	PRO	1741	25.074	-1.093	-6.237	1.00	17.82
MOTA	2016	CA	PRO	1741	23.763	-2.695	-4.980	1.00 2	
MOTA	2017	CB	PRO	1741	22.891	-1.554	-5.526	1.00	
MOTA	2018	CG	PRO	1741	23.866	-0.419	-5.647	1.00	
MOTA	2019	С	PRO	1741	23.189	-4.074	-5.343	1.00 2	
MOTA	2020	0	PRO	1741	22.700	-4.788	-4.462	1.00 2	
MOTA	2021	N	SER	1742	23.335	-4.473	-6.615	1.00 2	
ATOM	2022	CA	SER	1742	22.826	-5.754	-7.119	1.00 2	

AT	OM 2023	CB SER	1742	22.05
AT		OG SER	1742	24.234 -5.808 -8.641 1.00 23.67
AT		C SER	1742	22 524 -5.891 -9.023 1.00 26.64
AT		O SER	1742	-5.524 -6.545 1.00 23 00
ATO	- 42,	N GLN	1743	24 710
ATO		CA GLN	1743	-1.743 -0.782 -5.997 1.00 23 62
ATC	OM 2029	CB GLN	1743	-7.895 -5.416 1.00 23 26
ATC	-,	CG GLN	1743	$\frac{20.333}{1.00} = \frac{7.754}{5.702} = \frac{1.00.34}{1.00} = \frac{3.75}{1.00}$
ATO	M 2031	CD GLN	1743	-7.828 -7.170 1 00 23 04
ATO	M 2032	OE1 GLN	1743	26.684 -9.076 -7.810 1 00 24 02
ATO		NE2 GLN	1743	27.176 -10.178 -7.584 1.00 21 07
ATO		C GLN	1743	25.647 -8.907 -8.625 1.00 22 66
ATO		_	1743	-3.927 1.00 23 95
ATO			1744	25.744 -9.083 -3.366 1 00 25 26
ATO			1744	24.458 -7.240 -3.290 1.00 22 50
MOTA			1744	-1.395 -1.868 1.00 21 65
ATOM			1744	23.635 -6.087 -1.277 1.00 21 22
ATOM		GD	1744	24.623 -4.962 -1.342 1.00 21.62
ATOM	2041	1777	1744	24.013 -3.656 -0.863 1 00 19 06
ATOM			1744	24.869 -2.563 -1.318 1.00 24 44
ATOM	2043		.744	-1.322 -1.564 1.00 22 49
ATOM			744	-1.378 1.00 18 95
ATOM	2045		744	-0.438 -2.034 1.00 22 10
ATOM	-510 (	_	744	-0.4/0 -1.712 1.00 22 45
ATOM			745	-2.503 -8.772 -2.654 1.00 25 62
ATOM	2048 (		745	23.003 -9.139 -0.559 1 00 21 70
ATOM	2049 C		745	0.563 1.00 21.02
ATOM	2050 C	Th	745	-0.362 1.00 20 90
ATOM	2051 C		745	0.919 1.00 21 12
ATOM	2052 C		745	1.676 1.00 19 86
ATOM	2053 O		745	20 600 -9.485 -0.146 1.00 22.18
ATOM	2054 N		46	10.545 0.128 1.00 23.04
ATOM	2055 C		46	10.236 -0.297 1.00 19.31
ATOM	2056 CI		46	17 305 -9.689 -0.085 1.00 19.12
ATOM		31 THR 17	46	17 299 11 257
ATOM		32 THR 17	46	17 668 10 000 -0.886 1.00 22.54
ATOM	2059 C	THR 17	46	17 961 0 002 -2.479 1.00 22.97
ATOM ATOM	2060 O	THR 17	46	18.676 -10.733
ATOM	2061 N	PHE 17	47	16.884 -9.303
	2062 CA		17	16 456 0 570
ATOM	2063 CB		17	15 352 0 703
ATOM	2064 CG		17	15 872 7 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
ATOM		1 PHE 174	17	16 622 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ATOM		2 PHE 174	7	15 611 6 010
MOTA	2067 CE:	1 PHE 174	7	17 124 5 2.293 1.00 22.97
ATOM	2068 CE2	PHE 174	7	16 111 4 222
ATOM	2069 CZ	PHE 174	7	16 862 4 991 3.646 1.00 17.14
ATOM	2070 C	PHE 174		15 992 11 122
ATOM	2071 0	PHE 174		16 189 11 70-
ATOM	2072 N	LYS 174	8	15 420 13 60-
ATOM	2073 CA	LYS 174		14 971 12 97
ATOM	2074 CB	LYS 174		14 344 13 22
				14.344 -13.327 0.782 1.00 26.89
2005 (				

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ATOM	2075	CG	LYS	1748	14.061	-14.793	0.583	1.00	31.07
ATOM	2076	CD	LYS	1748	13.714	-15.064	-0.861	1.00	37.82
ATOM	2077	CE	LYS	1748	13.231	-16.493	-1.068	1.00	44.36
MOTA	2078	NZ	LYS	1748	12.027	-16.782	-0.235	1.00	50.16
ATOM	2079	С	LYS	1748	16.160	-13.949	2.393	1.00	27.27
ATOM	2080	0	LYS	1748	16.067	-14.877	3.202	1.00	27.87
ATOM	2081	N	GLN	1749	- 17.288	-13.674	1.730	1.00	25.64
ATOM	2082	CA	GLN	1749	18.507	-14.457	1.903	1.00	24.32
ATOM	2083	CB	GLN	1749	19.608	-13.938	0.983	1.00	28.87
MOTA	2084	CG	GLN	1749	19.343	-14.049	-0.496	1.00	36.24
ATOM	2085	CD	GLN	1749	20.437	-13.374	-1.318	1.00	41.30
MOTA	2086	OE1	GLN	1749	20.173	-12.422	-2.044	1.00	38.35
MOTA	2087	NE2	GLN	1749	21.683	-13.861	-1.190	1.00	45.38
ATOM	2088	С	GLN	1749	19.002	-14.310	3.346	1.00	22.89
ATOM	2089	0	GLN	1749	19.302	-15.305	4.008	1.00	22.55
ATOM	2090	N	LEU	1750	19.114	-13.064	3.813	1.00	20.89
ATOM	2091	CA	LEU	1750	19.570	~12.776	5.167	1.00	21.44
ATOM	2092	CB	LEU	1750	19.471	-11.282	5.462	1.00	19.53
ATOM	2093	CG	LEU	1750	20.432	-10.400	4.663	1.00	19.14
ATOM	2094	CD1	LEU	1750	20.069	-8.919	4.816	1.00	14.53
ATOM	2095	CD2	LEU	1750	21.863	-10.685	5.106	1.00	16.18
ATOM	2096	С	LEU	1750	18.776	-13.538	6.208	1.00	22.98
ATOM	2097	0	LEU	1750	19.335	-14.057	7.183	1.00	
ATOM	2098	N	VAL	1751		-13.586	6.020	1.00	23.48
ATOM	2099	CA	VAL	1751	16.610	-14.292	6.945	1.00	23.21
MOTA	2100	CB	VAL	1751	15.132	-14.075	6.590	1.00	
ATOM	2101	CG1	VAL	1751	14.268	-15.008	7.375	1.00	21.67
MOTA	2102	CG2	VAL	1751	14.730	-12.649	6.929	1.00	20.32
MOTA	2103	С	VAL	1751	16.974	-15.774	6.990	1.00	26.13
MOTA	2104	0	VAL	1751	17.030	-16.379	8.058	1.00	26.35
ATOM	2105	N	GLU	1752	17.260	-16.348	5.831	1.00	30.05
ATOM	2106	CA	GLU	1752	17.632	-17.747	5.778	1.00	32.54
MOTA	2107	CB	GLU	1752	17.695	-18.221	.4.338	1.00	38.54
MOTA	2108	CG	GLU	1752	16.322	-18.226	3.673	1.00	50.06
MOTA	2109	CD	GLU	1752	16.333	-18.759	2.247	1.00	56.55
MOTA	2110	OE1	GLU	1752	15.365	-18.480	1.507	1.00	61.63
MOTA	2111	OE2	GLU	1752	17.303	-19.466	1.875	1.00	59.57
MOTA	2112	C	GLU	1752	18.974	-17.965	6.486	1.00	31.62
MOTA	2113	0	GLU	1752	19.113	-18.858	7.322	1.00	29.63
MOTA	2114	N	ASP	1753	19.938	-17.103	6.193	1.00	30.74
MOTA	2115	CA	ASP	1753	21.246	-17.211	6.807	1.00	31.00
MOTA	2116	CB	ASP	1753	22.209	-16.181	6.203	1.00	31.47
ATOM	2117	CG	ASP	1753	22.445	-16.390	4.710	1.00	35.82
MOTA	2118	OD1	ASP	1753	22.396	-17.549	4.248	1.00	36.78
ATOM	2119	OD2	ASP	1753	22.671	-15.396	3.992	1.00	41.04
MOTA	2120	С	ASP	1753	21.158	-17.058	8.314	1.00	28.94
ATOM	2121	0	ASP	1753	21.597	-17.933	9.059	1.00	29.91
ATOM	2122	N	LEU	1754	20.526	-15.984	8.764	1.00	
ATOM	2123	CA	LEU	1754	20.386	-15.731	10.199	1.00	26.88
ATOM	2124	CB	LEU	1754	19.724	-14.372	10.457	1.00	
MOTA	2125	CG	LEU	1754	20.737	-13.269	10.154	1.00	
ATOM	2126	CD1	LEU	1754	20.074	-11.886	9.995	1.00	14.83

AT		1/34	21 921 12 22
AT		C LEU 1754	10.615 -13.308 11.240 1.00 16.39
ATO		O LEU 1754	20.030 -16.861 10.896 1.00 29.18
ATO		N ASP 1755	18 639 17 400
ATO		CA ASP 1755	17 000 17 10.238 1.00 31.65
ATC		CB ASP 1755	16 722 18.517 10.822 1.00 31.78
ATC		CG ASP 1755	15 R76 10 000 9.928 1.00 34.57
ATC		OD1 ASP 1755	15.410 19.997 10.533 1.00 38.29
ATO		OD2 ASP 1755	15 685 23 844 11.677 1.00 45.68
ATO		C ASP 1755	10.003 -21.031 9.878 1.00 43.09
ATO		O ASP 1755	18 665 20 103 11.034 1.00 33.50
ATO		N ARG 1756	10.730 120.428 12.025 1.00 34.39
ATO		CA ARG 1756	20 700 - 19.907 10.107 1.00 35.51
ATO		CB ARG 1756	21 417 22 1004 10.169 1.00 35.33
ATON		CG ARG 1756	22 522 22 10
ATON		CD ARG 1756	22.101 8.759 1.00 40.99
ATOM		NE ARG 1756	23 676 22 27 7.376 1.00 44.60
ATOM	_	CZ ARG 1756	24 795 20 227 6.916 1.00 49.55
ATOM		NH1 ARG 1756	25 556 20 227
ATOM		NH2 ARG 1756	35 155 120.937 8.266 1.00 53.25
ATOM	,	C ARG 1756	21 719 20 75
ATOM	0	O ARG 1756	22 000 21 525
ATOM		N ILE 1757	22 244 10 535
ATOM	_	CA ILE 1757	23 242 10 153
ATOM		CB ILE 1757	23 847 17 772
ATOM	<b>.</b> .	CG2 ILE 1757	24 915 17 405
MOTA MOTA	<b>.</b> .	CG1 ILE 1757	24 481 12 757
ATOM		CD1 ILE 1757	24 812 16 33.64
ATOM	2155 C	1/5/	22 673 10 11
ATOM	2156 C	1/3/	23 282 30 76
ATOM	2157 N	1102 1738	21 499 19 600
ATOM		A VAL 1758	20 854 . 10 500
ATOM	2159 C		19 378 -10 30.
ATOM		G1 VAL 1758	18 715 10 10
ATOM		G2 VAL 1758	19 309 16 57
ATOM	2162 C	/50	20 005 10 5-1
ATOM	2163 0	11.12 17.50	21 402 20 43.92
ATOM	2164 N 2165 C		20 370 20 000
ATOM			20.325 -22 354 15 -23.96
ATOM			19 653 23 307
ATOM	22.5-	ALA 1759	21 607 20 000
ATOM		ALA 1759	21 700 22 22
ATOM		LEU 1760	22 750 20
ATOM	2170 CA 2171 CB		24 005 22 21
ATOM			24 888 22 22
ATOM			24.279 -23.645 13.053 1.00 51.22
ATOM		1 LEU 1760	25.016 -23.279 11.778 1.00 55.38
ATOM	_	2 LEU 1760	24 327 25 36.19
ATOM	0 = = =	LEU 1760	24.811 -22.118 16.578 1.00 47.00
ATOM		LEU 1760	25.935 -22.432 16 986 1 00 44 55
ATOM		THR 1761	24.181 -21.031 17.004 1.00 49.83
	2178 CA	THR 1761	24 701 20 200
			24.791 -20.166 17.987 1.00 50.15



ATOM	2179	CB	THR	1761	24.309	-18.707	17.811	1.00 49.78
ATOM	2180	OG1	THR	1761	24.650	-18.262	16.489	1.00 49.83
ATOM	2181	CG2	THR	1761	24.997	-17.793	18.809	1.00 49.37
ATOM	2182	C	THR	1761	24.643	-20.655	19.426	1.00 51.84
ATOM	2183	0	THR	1761	23.565	-21.064	19.866	1.00 51.38
ATOM	2184	N	SER	1762	25.761	-20.622	20.143	1.00 53.45
ATOM	2185	CA	SER	1762	25.835	-21.042	21.533	1.00 53.79
ATOM	2186	CB	SER	1762	27.301	-21.039	21.969	1.00 58.33
MOTA	2187	OG	SER	1762	27.502	-21.759	23.173	1.00 63.27
MOTA	2188	C	SER	1762	25.033	-20.081	22.403	1.00 50.43
MOTA	2189	0	SER	1762	25.193	-18.856	22.301	1.00 48.42
MOTA	2190	N	ALA	461	79.680	25.808	14.502	1.00 57.40
ATOM	2191	ÇA	ALA	461	79.609	24.651	13.610	1.00 53.47
ATOM	2192	CB	ALA	461	78.307	23.875	13.860	1.00 54.34
ATOM	2193	С	ALA	461	79.707	25.105	12.151	1.00 49.53
MOTA	2194	0	ALA	461	79.739	24.289	11.243	1.00 48.04
MOTA	2195	N	ALA	462	79.814	26.417	11.957	1.00 46.57
MOTA	2196	CA	ALA	462	79.919	27.014	10.634	1.00 43.66
MOTA	2197	CB	ALA	462	80.034	28.532	10.750	1.00 43.87
MOTA	2198	C	ALA	462	81.074	26.461	9.806	1.00 39.75
MOTA	2199	0	ALA	462	80.869	26.036	8.673	1.00 36.18
MOTA	2200	N	TYR	463	82.279	26.449	10.383	1.00 37.82
ATOM	2201	CA	TYR	463	83.477	25.959	9.686	1.00 36.88
ATOM	2202	СВ	TYR	463	84.615	26.968	9.7€5	1.00 39.12
ATOM	2203	CG	TYR	463	. 84.372	28.176	8.894	1.00 45.68
ATOM	2204	CD1	TYR	463	84.071	29.422	9.456	1.00 46.07
ATOM	2205	CEl	TYR	463	83.783	30.518	8.652	1.00 48.07
ATOM	2206	CD2	TYR	463	84.384	28.064	7.501	1.00 47.80
MOTA	2207	CE2	TYR	463	84.096	29.154	6.690	1.00 45.55
MOTA	2208	CZ	TYR	463	83.796	30.372	7.271	1.00 47.44
MOTA	2209	OH	TYR	463	83.491	31.442	6.476	1.00 49.77
ATOM	2210	C	TYR	463	83.988	24.579	10.024	1.00 34.97
ATOM	2211	0	TYR	463	84.605	23.947	9.175	1.00 35.48
MOTA	2212	N	GLU	464	83.761	24.109	11.244	1.00 34.33
ATOM	2213	CA	GLU	464	84.224	22.769	11.630	1.00 36.96
MOTA	2214	CB	GLU	464	. 85.725	22.790	11.901	1.00 41.01
MOTA	2215	CG	GLU	464	86.123	23.764	12.991	1.00 45.91
MOTA	2216	CD	GLU	464	87.619	24.009	13.075	1.00 53.97
MOTA	2217	OE1	GLU	464	88.013	24.922	13.835	1.00 58.84
ATOM	2218	OE2	GLU	464	88.400	23.311	12.383	1.00 56.78
ATOM	2219	C	GLU	464	83.517	22.294	12.875	1.00 34.98
ATOM	2220	0	GLU	464	83.252	23.106	13.763	1.00 35.30
ATOM	2221	N	LEU	465	83.193	21.003	12.939	1.00 33.52
ATOM	2222	CA	LEU	465	82.527	20.449	14.121	1.00 35.65
MOTA	2223	CB	LEU	465	81.520	19.348	13.762	1.00 32.97
MOTA	2224	CG	LEU	465	80.488	19.538	12.651	1.00 33.16
MOTA	2225	CD1		465	79.356	18.544	12.911	1.00 27.30
MOTA	2226	CD2	LEU	465	79.983	20.981	12.596	1.00 29.96
ATOM	2227	C	LEU	465	83.572	19.862	15.058	1.00 38.14
MOTA	2228	0	LEU	465	84.707	19.573	14.642	1.00 35.58
MOTA	2229	N	PRO	466	83.215	19.684	16.338	1.00 39.91
ATOM	2230	CD	PRO	466	81.929	20.073	16.942	1.00 42.38

ATO			A PRO	466	84.	118 19.12	06 17 24	
ATO			B PRO	466	83.			
ATO			G PRO	466	82.			02
ATO			PRO	466	84.4			
ATOM		35 O	PRO		83.6		_	
ATON		36 N	GLU		85.6		_	10.04
ATOM		37 C.	A GLU		86.1			
ATOM		8 C	B GLU		87.5		_	
ATOM		9 C	GLU		88.0			
ATOM		0 CI	GLU	467	89.3			
ATOM	224	1 OF	E1 GLU		90.1			1.00 63.95
ATOM				467	89.6			1.00 62.08
ATOM	224	3 C	GLU	467	85.8			1.00 66.76
ATOM	224	4 0	GLU	467	85.9	_		1.00 44.81
ATOM	224	5 N	ASP	468				1.00 45.53
ATOM	224	CA		468	85.5			1.00 43.85
ATOM	224	7 CB		468	85.39			1.00 43.44
ATOM	2248	G CG		468	83.81			1.00 43.33
ATOM	2249		1 ASP	468	83.61		·	1.00 44.52
ATOM	2250		2 ASP	468	82.45			1.00 48.19
ATOM	2251		ASP	468	84.55 85.88			1.00 42.43
ATOM	2252	O	ASP	468	85.15		18.299	1.00 42.37
ATOM	2253	N	PRO	469	87.19		17.669	1.00 43.22
ATOM	2254	CD	PRO	469	88.16		18.433	1.00 40.72
ATOM	2255	CA	PRO	469			19.045	1.00 40.30
ATOM	2256	CB	PRO	469	87.86		17.909	1.00 39.00
ATOM	2257	CG	PRO	469	89.22	_	18.570	1.00 39.03
MOTA	2258	C	PRO	469	89.48	- <del>-</del>	18.551	1.00 38.11
ATOM	2259	0	PRO	469	87.17	_	18.229	1.00 39.37
ATOM	2260	N	ARG	470	87.23! 86.491		17.442	1.00 39.27
ATOM	2261	CA	ARG	470	85.814		19.371	1.00 39.93
ATOM	2262	CB	ARG	470	85.03(		19.770	1.00 42.32
ATOM	2263	CG	ARG	470	85.766		21.062	1.00 46.12
ATOM	2264	CD	ARG	470	84.839	-		1.00 50.76
ATOM	2265	NE	ARG	470	83.649	_		1.00 52.76
ATOM	2266	CZ	ARG	470	82.770			1.00 54.47
MOTA	2267	NH1		470	82.770			1.00 59.36
ATOM	2268	NH2		470	81.712			1.00 61.19
ATOM	2269	С	ARG	470	84.814			1.00 62.88
ATOM	2270	0	ARG	470	84.670	6.896		1.00 42.79
ATOM	2271	N	TRP	471	84.139	5.700		L.00 45.63
ATOM	2272	CA	TRP	471	83.100	7.844		L.00 41.98
ATOM	2273	CB	TRP	471	81.844	7.542		1.00 38.34
ATOM	2274		TRP	471	81.195	8.307		00 35.68
ATOM	2275	CD2		471	80.388	7.794	18.670	00 37.42
ATOM	2276	CE2		471	79.961	6.614	18.772 1	.00 37.19
MOTA	2277	CE3		471	79.987	6.513	20.112 1	.00 36.99
ATOM	2278	CD1		471			17.855 1	.00 37.80
ATOM	2279	NE1		471	81.223 80.486		19.923 1	.00 33.34
ATOM	2280	CZ2		471	79.150			.00 34.46
ATOM		CZ3		471	79.130			.00 38.31
MOTA		CH2		471				.00 36.97
					78.772	4.506	19.638 1	.00 36.14

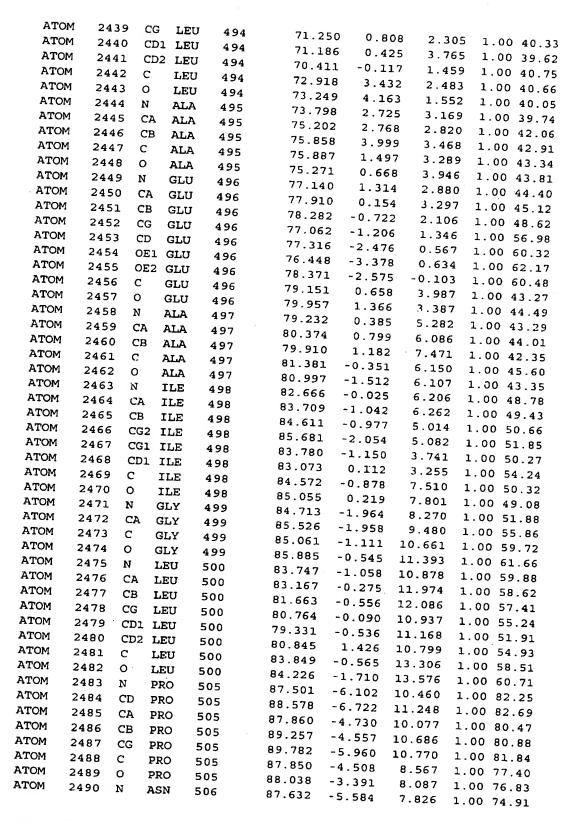


ATOM	2283	C	TRP	471	83.409	7.830	15.641	1.00 38.26
MOTA	2284	0	TRP	471	82.655	7.430	14.749	1.00 38.72
MOTA	2285	N	GLU	472	84.478	8.569	15.397	1.00 37.71
ATOM	2286	CA	GLU	472	84.839	8.951	14.041	1.00 38.43
MOTA	2287	CB	GLU	472	86.014	9.924	14.087	1.00 37.56
ATOM	2288	CG	GLU	472	86.146	10.835	12.871	1.00 37.26
ATOM	2289	CD	GLU	472	84.930	11.728	12.625	1.00 39.02
MOTA	2290	OE1	GLU	472	84.361	12.301	13.571	1.00 40.26
ATOM	2291		GLU	472	84.568	11.879	11.445	1.00 39.35
ATOM	2292	С	GLU	472	85.135	7.806	13.069	1.00 38.32
ATOM	2293	0	GLU	472	85.872	6.875	13.386	1.00 38.11
ATOM	2294	N	LEU	473	84.535	7.884	11.883	1.00 38.44
MOTA	2295	CA	LEU	473	84.775	6.893	10.848	1.00 37.19
ATOM	2296	CB	LEU	473	83.505	6.112	10.511	1.00 35.38
ATOM	2297	CG	LEU	473	83.805	4.910	9.599	1.00 36.49
MOTA	2298	CD1	LEU	473	84.365	3.748	10.406	1.00 34.47
MOTA	2299		LEU	473	82.556	4.452	8.859	1.00 37.55
MOTA	2300	С	LEU	473	85.283	7.623	9.601	1.00 38.21
ATOM	2301	0	LEU	473	84.696	8.631	9.187	1.00 38.52
ATOM	2302	N	PRO	474	86.412	7.156	9.025	1.00 37.74
ATOM	2303	CD	PRO	474	87.292	6.107	9.568	1.00 36.38
ATOM	2304	CA	PRO	474	87.010	7.753	7.824	1.00 36.91
ATOM	2305	CB	PRO	474	88.233	6.865	7.587	1.00 34.65
ATOM	2306	CG	PRO	474	88.620	6.477	8.967	1.00 32.99
ATOM	2307	C	PRO	474	86.036	7.663	6.660	1.00 38.15
ATOM	2308	0	PRO	474	85.536	6.578	6.362	1.00 38.24
ATOM	2309	N	ARG	475	85.793	8.784	5.981	1.00 38.90
MOTA	2310	CA	ARG	475	84.846	8.802	4.863	1.00 41.23
ATOM	2311	CB	ARG	475	84.743	10.206	4.258	1.00 38.36
ATOM	2312	CG	ARG	475	84.311	11.271	5.267	1.00 35.30
ATOM	2313	CD	ARG	475	84.282	12.691	4.679	1.00 35.23
ATOM ATOM	2314 2315	NE CZ	ARG ARG	475	83.850	13.658	5.679	1.00 27.27
ATOM	2315		ARG	475	82.585	13.859	6.011	1.00 25.77
ATOM	2317		ARG	475 475	81.630 82.286	13.181	5.402	1.00 25.09
ATOM	2317	C	ARG	475 475	85.101	14.639	7.047	1.00 25.24
ATOM	2319	0	ARG	475	84.160	7.745 7.212	3.791 3.204	1.00 42.43
ATOM	2320	N	ASP	476	86.359	7.381	3.594	1.00 44.69
ATOM	2321	CA	ASP	476	86.690	6.384	2.583	1.00 48.37
ATOM	2322	CB	ASP	476	88.197	6.371	2.319	1.00 40.37
ATOM	2323	CG	ASP	476	88.988	5.925	3.521	1.00 56.56
ATOM	2324		ASP	476	89.299	4.718	3.613	1.00 59.72
ATOM	2325		ASP	476	89.294	6.779	4.376	1.00 53.72
ATOM	2326	C	ASP	476	86.210	4.988	2.973	1.00 49.50
ATOM	2327	0	ASP	476	86.204	4.074	2.145	1.00 43.30
ATOM	2328	N	ARG	477	85.852	4.814	4.241	1.00 48.26
ATOM	2329	CA	ARG	477	85.357	3.525	4.732	1.00 47.16
ATOM	2330	CB	ARG	477	85.909	3.252	6.126	1.00 47.16
ATOM	2331	CG	ARG	477	87.325	2.723	6.088	1.00 53.76
ATOM	2332	CD	ARG	477	88.043	2.898	7.406	1.00 58.02
ATOM	2333	NE	ARG	477	87.394	2.213	8.517	1.00 58.02
ATOM	2334	cz	ARG	477	87.810	2.213	9.776	1.00 63.35
					0010	/	5.770	00 05.35



3.77	BOM .										
		2335	NH1		477	88.8	75 2				
	OM 2	2336	NH2	ARG	477	87.1			081	1.00	64.92
		2337	C	ARG	477	83.8			738	1.00	66.00
		338	0	ARG	477	83.2			740	1.00	45.38
AT	_	339	N	LEU	478		_	. • •		1.00	43.67
AT		340	CA	LEU	478	83.1			026	1.00	42.09
ATO		341	CB :	LEU	478	81.72			951	1.00	37.74
AT(		342	CG 1	LEU	478	81.19	_		349	1.00	32.19
ATO	OM 2.	343	CD1 1		478	79.67			73	1.00	30.21
ATO	DM 2:	344	CD2 I		478	79.14			83 ;	1.00	22.82
ATC	DM 2:	345		EU	478	79.31		35 5.4			34.82
ATC	M 23	346	_	EU	478	81.32		2.5		1.00	38.75
ATO				AL	479	81.81		9 1.9			40.60
ATO				AL		80.47		3 1.9		. 00	38.78
ATO				AL	479	80.02		8 0.5			37.97
ATO			CG1 V		479	80.35		5 -0.3		00	37.97 36.36
ATO			CG2 V	M.I.	479	79.83	7 3.09				
ATO					479	81.868	2.62				33.55
ATON			-	AL	479	78.523	4.29			.00	33.76
ATON		_ `	_	AL.	479	77.750	3.38			.00 3	37.83
ATOM		_			480	78.127	5.542		_	.00 3	
ATOM			CA LE		480	<sup>7</sup> 6.723	5.942		_	.00 3	9.32
ATOM			B LE		480	76.630	7.458			. OC 3	8.41
ATOM			G LE		480	77.287	8.226			.00 3	8.29
ATOM			D1 LE		480	77.098	9.730			00 3	7.99
ATOM			D2 LE		480	76.666	7.785			00 3	4.00
ATOM		_			480	75.893	5.287			00 3	2.79
ATOM	_	_			480	76.315	5.205			00 38	3.24
ATOM					481	74.672	4.896			00 39	∍.11
ATOM	236				481	73.811	4.223	-0.394		00 36	5.70
ATOM	236 236	_	GL		481	72.417	4.782	-1.357		00 36	5.53
ATOM		_	GL		481	72.159	5.961	-1.524		00 37	7.61
ATOM	2366	_	LYS	;	482	71.484	3.913	-1.277		00 40	.02
ATOM	2361				482	70.099	4.313	-1.911		00 37	. 52
ATOM	2368				482	69.243	3.104	-2.153		00 39	. 89
ATOM	2369		LYS		482	69.447	5.028	-2.551		0 42	. 44
ATOM	2370		LYS		182	69.538	4.589	-0.984		0 41	.25
ATOM	2371		PRO		183	68.779	6.156	0.163	1.0	0 42	.22
ATOM	2372		PRO	4	183	68.643	6.876	-1.263	1.0	0 41	. 71
ATOM	2373		PRO	4	83	68.118	6.889	-2.537		0 41	
ATOM	2374	CB	PRO	4	83	67.606	8.146	-0.193	1.0	0 42	. 72
	2375		PRO	4	83	67.425	7.713	-0.906	1.0	0 41.	.26
ATOM ATOM	2376	C	PRO	4	83	66.999	6.061	-2.290	1.0	0 40.	16
	2377	0	PRO	4	83	66.306	5.314	0.429	1.00	0 44.	69
ATOM	2378	N.	LEU	4	84	66.883		-0.262	1.00	9 45.	26
ATOM	2379	CA	LEU		84	65.872	6.163	1.751	1.00	45.	34
ATOM	2380	CB	LEU		84	66.494	5.450	2 512	1.00	47.	34
ATOM	2381	CG	LEU		84	67.517	4.793	3.746	1.00	42.	40
ATOM	2382	CD1	LEU		34	68.208	3.668	3.535	1.00	39.	50
ATOM	2383	CD2	LEU		34	66.861	3.337	4.828	1.00	33.	64
ATOM	2384	С	LEU	48			2.419	3.003	1.00	33.4	44
ATOM	2385	0	LEU	4 6		64.733	6.391	2.927	1.00	52.1	14
MOTA	2386	N	GLY	48		63.611	5.941	3.142	1.00	53.6	54
					-	65.013	7.697	3.025	1.00	55.2	25
										_	

MOTA	2387	CA	GLY	485	63.982	8.653	3.427	1.00 58.76
MOTA	2388	С	GLY	485	64.441	10.104	3.503	1.00 60.58
ATOM	2389	0	GLY	485	65.640	10.376	3.600	1.00 61.49
ATOM	2390	N	ALA	486	63.490	11.032	3.489	1.00 61.46
MOTA	2391	CA	ALA	486	63.791	12.458	3.545	1.00 63.24
MOTA	2392	CB	ALA	486	63.847	13.035	2.126	1.00 64.42
ATOM	2393	C	ALA	486	62.730	13.179	4.355	1.00 63.86
ATOM	2394	0	ALA	486	61.655	12.633	4.599	1.00 65.24
MOTA	2395	N	GLY	487	63.022	14.404	4.768	1.00 63.89
MOTA	2396	CA	GLY	487	62.054	15.158	5.538	1.00 64.30
ATOM	2397	С	GLY	487	62.431	16.617	5.623	1.00 65.34
MOTA	2398	0	GLY	487	63.071	17.154	4.718	1.00 65.98
ATOM	2399	N	ALA	488	. 62.023	17.259	6.711	1.00 66.16
ATOM	2400	CA	ALA	488	62.317	18.666	6.934	1.00 66.71
ATOM	2401	CB	ALA	488	61.647	19.132	8.219	1.00 70.05
MOTA	2402	С	ALA	488	63.828	18.844	7.027	1.00 66.55
ATOM	2403	0	ALA	488	64.432	18.547	8.063	1.00 65.59
ATOM	2404	N	PHE	489	64.430	19.228	5.904	1.00 65.54
MOTA	2405	CA	PHE	489	65.875	19.457	5.807	1.00 65.40
ATOM	2406	CB	PHE	489	66.244	20.775	6.498	1.00 67.06
ATOM	2407	С	PHE	489	66.773	18.296	6.311	1.00 64.01
ATOM	2408	0	PHE	489	67.942	18.502	6.651	1.00 62.51
ATOM	2409	N	GLY	490	66.234	17.075	6.288	1.00 61.41
ATOM	2410	CA	GLY	490	66.974	15.901	6.724	1.00 55.89
ATOM	2411	C	GLY	490	66.858	14.821	5.667	1.00 53.58
ATOM	2412	0	GLY	490	65.825	14.703	5.000	1.00 54.22
ATOM	2413	N	GLN	491	67.899	14.006	5.543	1.00 51.23
ATOM	2414	CA	GLN	491	67.966	12.934	4.556	1.00 47.90
MOTA	2415	CB	GLN	491	68.823	13.445	3.387	1.00 50.09
ATOM	2416	CG	GLN	491	. 68.979	12.529	2.183	1.00 56.77
ATOM	2417	CD	GLN	491	69.945	13.115	1.161	1.00 60.83
ATOM ATOM	2418	OE1		491	70.283	14.292	1.218	1.00 65.11
ATOM	2419 2420	NE2	GLN GLN	491 491	70.411	12.284	0.232	1.00 63.81
ATOM	2421	0	GLN		68.597	11.673	5.190	1.00 45.27
ATOM	2422	N	VAL	491 492	69.507	11.758	6.014	1.00 45.41
ATOM	2423	CA	VAL	492	68.112 68.624	10.503	4.805	1.00 41.69
ATOM	2424	CB	VAL	492	67.583	9.245 8.528	5.325	1.00 39.95
ATOM	2425		VAL	492	68.117	7.168	6.230 6.701	1.00 41.77 1.00 39.86
ATOM	2426		VAL	492	67.226	9.399	7.421	1.00 39.86
ATOM	2427	C	VAL	492	68.911	8.348	4.126	1.00 42.87
ATOM	2428	o	VAL	492	68.025	8.114	3.301	1.00 38.86
ATOM	2429	N	VAL	493	70.141	7.862	4.010	
MOTA	2430	CA	VAL	493	70.481	6.994	2.895	1.00 36.01 1.00 37.55
ATOM	2431	СВ	VAL	493	71.471	7674		
ATOM	2432		VAL	493	71.128	9.137	1.889 1.709	1.00 38.65
ATOM	2433		VAL	493	72.929	7.498	2.318	1.00 37.08 1.00 39.03
ATOM	2434	C	VAL	493	71.071	5.678	3.371	1.00 39.03
ATOM	2435	0	VAL	493	71.645	5.599	4.456	1.00 38.61
ATOM	2436	N	LEU	494	70.899	4.637	2.572	1.00 39.75
ATOM	2437	CA	LEU	494	71.460	3.345	2.910	1.00 39.68
ATOM	2438	CB	LEU	494	70.748	2.241	2.310	1.00 40.98
						0.471	4.143	1.00 42.14



MOTA	2491	CA	ASN	506	87.572	-5.502	6.375	1.00 73.04
ATOM	2492	CB	ASN	506	88.632	-6.406	5.749	1.00 73.39
MOTA	2493	С	ASN	506	86.180	-5.938	5.929	1.00 71.75
ATOM	2494	0	ASN	506	85.918	-6.094	4.739	1.00 71.33
ATOM	2495	N	ARG	507	85.294	-6.124	6.905	1.00 69.66
ATOM	2496	CA	ARG	507	83.924	-6.534	6.638	1.00 66.59
ATOM	2497	CB	ARG	507	83.369	-7.329	7.819	1.00 69.86
ATOM	2498	С	ARG	507	83.048	-5.321	6.409	1.00 63.59
MOTA	2499	0	ARG	507	83.225	-4.291	7.070	1.00 64.09
ATOM	2500	N	VAL	508	82.126	-5.429	5.462	1.00 59.52
MOTA	2501	CA	VAL	508	81.217	-4.334	5.187	1.00 57.28
MOTA	2502	CB	VAL	508	80.905	-4.178	3.686	1.00 55.73
ATOM	2503		LAV	508	82.163	-3.952	2.922	1.00 57.01
ATOM	2504		VAL	508	80.184	-5.390	3.149	1.00 58.06
ATOM	2505	С	VAL	508	79.928	-4.614	5.935	1.00 57.10
ATOM	2506	0	VAL	508	79.483	-5. <b>75</b> 9	6.018	1.00 57.35
MOTA	2507	N	THR	509	79.345	-3.555	6.482	1.00 55.31
MOTA	2508	CA	THR	509	78.107	-3.652	7.227	1.00 50.14
MOTA	2509	CB	THR	509	78.329	-3.192	8.686	1.00 50.91
ATOM	2510	OG1		509	79.476	-3.851	9.227	1.00 49.20
ATOM	2511	CG2		509	77.123	-3.524	9.559	1.00 51.96
ATOM	2512	C	THR	509	77.140	-2.705	6.528	1.00 47.53
ATOM	2513	0	THR	509	77.485	-1.558	6.242	1.00 47.22
MOTA	2514	N	LYS	510	75.958	-3.191	6.191	1.00 45.64
ATOM	2515	CA	LYS	510	74.975	-2.333	5.551	1.00 44.44
ATOM	2516	СВ	LYS	510	73.861	-3.175	4.948	1.00 46.74
ATOM	2517	CG	LYS	510	73.008	-2.420	3.950	1.00 54.51
ATOM	2518	CD	LYS	510	73.463	-2.645	2.513	1.00 54.97
ATOM	2519	CE	LYS	510	72.846	-3.917	1.934	1.00 58.25
ATOM	2520	NZ	LYS	510	73.112	-5.150	2.740	1.00 58.33
ATOM .	2521	C	LYS	510	74.430	-1.470	6.696	1.00 42.75
MOTA	2522	0	LYS	510	74.053	-2.006	7.742	1.00 43.14
ATOM	2523	N	VAL	511	74.443	-0.149	6.531	1.00 38.63
ATOM ATOM	2524	CA	VAL	511	73.975	0.757	7.576	1.00 34.16
ATOM	2525	CB	VAL	511	75.161	1.399	8.333	1.00 35.66
ATOM	2526	CG1	VAL	511	75.922	0.340	9.100	1.00 31.46
ATOM	2527 2528	CG2 C	VAL VAL	511 511	76.098	2.100	7.357	1.00 35.08
ATOM	2529	0	VAL	511	73.116	1.873	7.024	1.00 31.58
ATOM	2530	N	ALA	512	72.962 72.542	1.984 2.687	5.818	1.00 33.18
ATOM	2531	CA	ALA	512	71.724	3.818	7.906	1.00 30.77
ATOM	2532	CB	ALA	512	70.382	3.774	7.484 8.145	1.00 28.58
ATOM	2533	C	ALA	512	72.487	5.075	7.905	1.00 26.09
ATOM	2534	0	ALA	512	72.996			1.00 29.94
ATOM	2535	N	VAL	513	72.556	5.151	9.031	1.00 29.90
ATOM	2536	CA	VAL	513	73.286	6.057 7.290	7.012	1.00 28.68
ATOM	2537	CB	VAL	513	74.439	7.503	7.280 6.269	1.00 28.26
ATOM	2538	CG1		513	75.213	8.730		1.00 26.92
ATOM	2539	CG2		513	75.353	6.308	6.618 6.238	1.00 25.26 1.00 25.10
MOTA	2540	C	VAL	513	72.383	8.526	7.230	1.00 25.10
ATOM	2541	0	VAL -	513	71.745	8.799	6.200	1.00 29.54
ATOM	2542	N	LYS	514	72.304	9.228	8.359	1.00 28.94
		••		~ 7.4	.4.507	J. 220	0.337	4.00 20.94

ATC	)M 2	543	CA	LYS	514		71 -								
ATO		544		LYS	514		71.5				8.4	81	1.0	0 28	.60
ATO		545		LYS	514		70.9				9.8		1.0	0 31	.19
ATO		46	_	LYS	514		69.9				10.3	28	1.0	0 31	.41
ATO		47		LYS	514		69.4		9.92		1.6	90		0 40	
ATO		48		LYS	514		68.4		8.89		2.2	22	1.00	48	. 93
ATO				LYS	514		67.1		8.86	_	1.4	75	1.00	57	. 07
ATO				YS	514		72.4		11.63		8.19	96	ι.ος	25.	. 53
ATOM	1 25			(ET	515		73.5		11.714		8.72	22 ]	1.00	20.	42
ATOM		52		ET	515		71.9		12.576		7.40	77 1	. 00	26.	63
ATOM		_		ET	515		72.6		13.762		7.00	8 1	. 00	27.	59
ATOM			_	ET	515		73.42		13.487		5.69	3 1	.00	28.	22
ATOM				ET	515		72.50		13.026		4.55	6 1	.00	28.	70
ATOM				ET	515		73.37		12.418		3.11	3 1	. 00	32.	30
ATOM		57 (		ET	515		73.94		10.803		3.71	5 1	.00	24.	88
ATOM	255	8 0		ET	515		71.68		14.880		.77	9 1	.00	28.	41
ATOM	255	9 N		EU	516		70.47		14.685		.88	9 1	.00	32.	15
ATOM	256	0 0		EU	516		72.20		16.056		.46	6 1	.00	29.	12
ATOM	256			ยับ	516		71.38		17.220	6	.18	0 1	. 00	29.	98
ATOM	256			ΞÜ	516		72.11		18.512	6	.593	3 1.	00	25.3	32
ATOM	256		D1 LE		516		72.45		18.767	8	.067	71.	00	26.6	50
ATOM	256	4 C	D2 LE		516		73.210		20.057	8	.190	1.	00	24.5	6
MOTA	256	5 C	LE		516		71.21		18.844		. 900	) 1.	00	22.7	5
ATOM	256	6 0	LE		516		71.092		17.274	4	. 674	1.	00	31.5	0
ATOM	2561	7 N			517		71.763		16.636	3	. 873	1.	00	32.9	7
ATOM	2568	C.			517		70.069		18.018		. 293	1.	00	33.2	9
ATOM	2569	CE			517		69.755		18.187		890	1.		32.2	
ATOM	2570	) co			517		68.246		18.363	2.	699	1.	00	36.3	4 -
ATOM	2571	CI			517		67.432		17.182	3.	192	1.	00 4	13.4	9
A'rom	2572	CE			517		66.172		16.940		356			3.9	
ATOM	2573	NZ	LY	3	517	•	65.088 63.902		17.984		581	1.0	00 5	8.7	L
ATOM	2574	_	LYS		517		70.520		17.740		704	1.0	00 5	59.37	7
ATOM	2575	0	LYS		517		70.320		19.455		507	1.0	00 3	1.31	Ļ
ATOM	2576	N	SEF		518		70.744		20.217		383			8.74	
ATOM	2577	CA	SER		518		71.486		.9.672		213			2.48	
ATOM	2578	CB	SER		518		71.611		0.840		714			3.52	
ATOM	2579	OG	SER		518		70.375		0.772 0.407	-0.8		1.0	0 3	2.98	
ATOM	2580	C	SER		518		70.896		2.189	-1.3				6.75	
ATOM	2581	0	SER	5	518		71.580		3.214	1.1				4.62	
ATOM	2582	N	ASP	5	19		69.624		2.193	1.0				4.57	
ATOM	2583	CA	ASP	5	19		68.943		3.422	1.4		1.0	0 3	5.47	
ATOM	2584	CB	ASP	5	19		67.529	2	3.422	1.8		1.0	0 36	5.10	
ATOM	2585	CG	ASP	5	19		66.668		2.258	1.2				3.11	
ATOM	2586		ASP	5	19		67.150		1.309	1.6		1.00	0 41	1.64	
ATOM	2587	OD2	ASP	5	19		65.478		2.250	2.2		1.00	41	70	
ATOM	2588	C	ASP	5	19		68.881		3.645	1.2		1.00			
ATOM	2589	0	ASP		19		68.266		1.602	3.3		1.00			
ATOM	2590	N	ALA	5	20		69.551		. 784	3.8		1.00	33	.39	
ATOM	2591	CA	ALA		20		69.561		784 2 . 895	4.19		1.00			
ATOM	2592	СВ	ALA		20		70.253		.687	5.60		1.00	32	.12	
	2593	С	ALA	52	20		70.242			6.20		1.00			
ATOM	2594	0	ALA	52	20		71.014	24		6.07		1.00	30	.91	
								-•		5.33	) T	1.00	30	. 57	

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ATOM	2595	N	THR	521	69.943	24.555	7.311	1.00	30.80
MOTA	2596	CA	THR	521	70.546	25.738	7.921	1.00	32.33
MOTA	2597	CB	THR	521	69.493	26.763	8.440	1.00	34.30
ATOM	2598	OG1	THR	521	68.817	26.242	9.598	1.00	35.14
ATOM	2599	CG2	THR	521	68.484	27.109	7.366	1.00	37.70
MOTA	2600	C	THR	521	71.418	25.312	9.098	1.00	33.11
ATOM	2601	0	THR	521	71.518	24.125	9.426	1.00	31.39
ATOM	2602	N	GLU	522	72.022	26.293	9.753	1.00	34.91
ATOM	2603	CA	GLU	522	72.882	26.048	10.901	1.00	39.44
ATOM	2604	CB	GLU	522	73.516	27.357	11.360	1.00	46.96
ATOM	2605	CG	GLU	522	74.550	27.220	12.488	1.00	59.20
ATOM	2606	CD	GLU	522	75.919	26.740	12.011	1.00	64.70
MOTA	2607		GLU	522	76.910	27.478	12.219	1.00	63.87
MOTA	2608		GLU	522	76.006	25.627	11.445	1.00	71.55
MOTA	2609	С	GLU	522	72.083	25.428	12.044	1.00	39.61
ATOM	2610	0	GLU	522	72.587	24.554	12.757	1.00	36.74
MOTA	2611	N	LYS	523	70.827	25.849	12.193	1.00	38.60
ATOM	2612	CA	LYS	523	69.970	25.327	13.252	1.00	37.77
ATOM	2613	СВ	LYS	523	68.628	26.053	13.273	1.00	44.52
MOTA	2614	CG	LYS	523	67.665	25.562	14.355	1.00	51.14
MOTA	2615	CD	LYS	523	66.380	24.983	13.756	1.00	57.39
ATOM	2616	CE	LYS	523	65.499	24.376	14.852	1.00	59.17
ATOM	2617	NZ	LYS	523	64.365	23.553	14.327	1.00	62.68
ATOM	2618	С	LYS	523	69.751	23.849	13.002	1.00	34.63
ATOM	2619	0	LYS	523	69.817	23.041	13.931	1.00	35.00
ATOM	2620	N	ASP	524	69.496	23.495	11.746	1.00	31.60
ATOM	2621	CA	ASP	524	69.293	22.100	11.367	1.00	29.05
MOTA	2622	CB	ASP	524	69.002	21.975	9.871	1.00	29.60
ATOM	2623	CG	ASP	524	67.695	22.626	9.472	1.00	31.90
MOTA	2624	OD1	ASP	524	66.666	22.368	10.130		38.83
ATOM	2625	OD2		524	67.687	23.383	8.485		29.79
ATOM	2626	C	ASP	524	70.558	21.317	11.696		28.02
ATOM	2627	0	ASP	524	70.494	20.201	12.212		28.12
MOTA	2628	N	LEU	525	71.709	21.899	11.378		28.32
ATOM	2629	CA	LEU	525	72.971	21.231	11.677		27.71
ATOM	2630	CB	LEU	525	74.173	22.085	11.257		22.53
ATOM	2631	CG	LEU	525	75.548	21.490	11.602		22.13
ATOM ATOM	2632	CD1		525	75.677	20.082	11.019		19.92
ATOM	2633 2634	CD2		525	76.673	22.401	11.147		18.60
ATOM	2635	C	LEU	525	73.007	20.952	13.162	1.00	
ATOM	2636	O N	LEU	525	73.227	19.817	13.577		29.73
ATOM	2637	N CA	SER	526	72.689	21.976	13.947	1.00	
ATOM	2638		SER	526	72.672	21.891	15.412	1.00	
		CB	SER	526	72.222	23.230	16.006	1.00	
ATOM ATOM	2639 2640	OG C	SER	526 526	71.966	23.147	17.397	1.00	
ATOM		C	SER	526 526	71.765	20.777	15.931	1.00	
ATOM	2641 2642	O N	SER	526	72.055	20.133	16.954	1.00	
		N CA	ASP	527	70.644	20.587	15.242	1.00	
ATOM ATOM	2643		ASP	527 527	69.681	19.558	15.601	1.00	
ATOM	2644		ASP	527	68.392	19.798	14.829	1.00	
ATOM	2645 2646		ASP	527 527	67.640	21.052	15.290	1.00	
A LON	2646	OD1	no r	527	68.016	21.662	16.320	1.00	∠6.80

ATC		47	OD2	ASP	527	66.6	۲0	22.4		_				
ATC	-	48		ASP	527	70.2				14.6				3.85
ATO			0 ;	ASP	527	70.0		18.1		15.3				8.34
ATO		50	N j	LEU	528	70.8		17.2		16.1				8.36
ATO			CA 1	LEU	528	71.4		17.9		14.1				9.50
ATO			CB I	LEU	528	71.9		16.6		13.8				0.48
ATO				ĿΕU	528	72.44		16.6		12.3		1.0	0 2.	7.89
ATO			CD1 I	EU	528	71.46		15.3		11.8				5.48
ATO		55 (	CD2 L	EU	528	72.72		14.15		12.1		1.00		
ATOM				EU	528	72.72		15.38		10.3		1.00	20	.23
ATON		57 (		EU	528	72.68		16.30		14.8		1.00		
ATOM		8	ı	LE	529	73.39		15.14		15.2		1.00		
ATOM		9 (	A I	LE	529	74.50		17.29		15.19		1.00		
ATOM		0 0	B I	LE	529	75.39		17.08		16.14		1.00	28	.88
ATOM		1 0	G2 I	LE	529	76.54		18.31		16.27	78 :	1.00	25	.69
ATOM		2 0	G1 II	LE	529	75.96		18.00		17.21		1.00	20	. 54
ATOM		3 C	D1 II		529	76.98		18.72		14.94	-	1.00	23	.71
ATOM	266				529	73.95		19.83		15.03	5 ]	1.00	24	.21
MOTA	266	5 0			529			16.76		17.53	3 1	1.00	31	. 52
ATOM	2666	5 N			530	74.439		15.85		1.8.21	3 1	.00		
MOTA	266	7 C			530	72.917		17.50		17.94	7 1	00	29.	79
ATOM	2668	3 CI			530	72.315		17.25		19.24	4 1	. 00	32.	03
ATOM	2669	9 00			530	71.176		18.239		19.49	2 1	.00	38.	91
ATOM	2670	) C	SE		530	70.266		18.231		18.41	2 1	.00		
ATOM	2671	. 0	SE		530	71.795		15.819		19.31	51	.00		
ATOM	2672	N	GL		531	71.921 71.185		15.154		20.35	3 1	.00		
ATOM	2673	CA	GL	U	531	70.671		15.350		18.23		.00	27.	18
MOTA	2674	CB			531	69.923		13.989		8.180	) 1	.00	27.	89
ATOM	2675	CG	GLI	ני	531	69.434		13.744		6.881		.00	31.	29
ATOM	2676	CD			531	68.717		12.324		€.769		.00	30.	43
ATOM	2677	OE	1 GL		531	68.293		12.040		5.486		.00		
ATOM	2678	OE			531	68.571		0.892		5.317		.00		
MOTA	2679	С	GLU		531	71.765		2.941		4.643		00		
MOTA	2680	0	GLU		531	71.604		2.929		8.348		00 2		
ATOM	2681	N	MET		532	72.851		1.986		9.119		00 2		
MOTA	2682	CA	MET		532	74.000		3.074		7.595		00 2	28.9	3
MOTA	2683	CB	MET		532	75.073		2.156 2.637		7.644		00 2		
ATOM	2684	CG	MET		532	76.458		2.034		5.659	1.	00 2	9.4	8
ATOM	2685	SD	MET		532	77.650				5.827		00 2		
ATOM	2686	CE	MET		532	77.831		2.692		5.582		00 3		
ATOM	2687	С	MET		32	74.571		4.373		.151	1.	00 2	0.1	0
MOTA	2688	0	MET		32	74.876				0.057	1.	00 2	9.0	6
ATOM	2689	N	GLU		33	74.640		1.053 3.289		.589	1.0	00 2	8.2	2
ATOM	2690	CA	GLU		33	75.150		3.388		.688	1.(	00 2	8.6	1
ATOM	2691	CB	GLU		33	75.340			21	.041	1.0	00 2	B.40	ס
ATOM	2692	CG	GLU		33	76.449		1.846		.429	1.0	00 2	9.34	1
ATOM	2693	CD	GLU		33	77.822		5.534		.640		00 3:		
ATOM	2694	OE1	GLU		33	78.242		.923		.892	1.0	0 3	5.10	)
ATOM	2695	OE2	GLU		33	78.490		.831		.067	1.0	0 31	7.36	5
ATOM	2696	C	GLU		33	74.211		.543		. 913	1.0	0 37	7.71	
ATOM	2697	0	GLU		33	74.651		.684		. 023	1.0	0 31	03	
ATOM	2698	N	MET		34			. 936 . 902		. 906	1.0	0 30	- 76	
							-2	. 302	21	. 860	1.0	0 31	.71	



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ATOM	2699	CA	MET	534	71.940	12.256	22.727	1.00 30.58
ATOM	2700	CB	MET	534	70.510	12.620	22.315	1.00 33.53
ATOM	2701	CG	MET	534	69.538	12.624	23.509	0.50 32.45
ATOM	2702	SD	MET	534	67.778	12.682	23.150	0.50 30.95
ATOM	2703	CE	MET	534	67.523	14.422	22.895	0.50 30.50
ATOM	2704	С	MET	534	72.158	10.752	22.616	1.00 28.44
ATOM	2705	0	MET	534	72.304	10.077	23.614	1.00 27.63
ATOM	2706	N	MET	535	72.216	10.232	21.395	1.00 30.00
ATOM	2707	CA	MET	535	72.448	8.800	21.176	1.00 29.38
ATOM	2708	CB	MET	535	72.626	8.483	19.690	1.00 25.41
ATOM	2709	CG	MET	535	71.395	8.753	18.893	1.00 25.06
ATOM	2710	SD	MET	535	71.468	7.917	17.344	1.00 27.17
ATOM	2711	CE	MET	535	71.439	9.227	16.247	1.00 33.70
ATOM	2712	C	MET	535	73.675	8.345	21.938	1.00 30.77
ATOM	2713	ō	MET	535	73.681	7.254	22.534	1.00 30.77
ATOM	2714	N	LYS	536	74.710	9.183	21.916	1.00 27.43
ATOM		CA	LYS	536			22.649	
	2715				75.937	8.889		1.00 34.05
ATOM	2716	CB	LYS	536	76.995	9.964	22.401	1.00 32.69
ATOM	2717	CG	LYS	536	77.719	9.838	21.073	1.00 28.00
ATOM	2718	CD	LYS	536	78.732	10.956	20.941	1.00 29.61
ATOM	2719	CE	LYS	536	79.242	11.124	19.514	1.00 26.58
ATOM	2720	NZ	LYS	536	80.020	12.389	19.460	1.00 22.22
ATOM	2721	C	LYS	536	75.652	8.769	24.145	1.00 34.80
ATOM	2722	0	LYS	536	76.004	7.763	24.750	1.00 34.44
ATOM	2723	N	MET	537	74.958	9.749	24.716	1.00 34.66
MOTA	2724	CA	MET	537	74.634	9.724	26.131	1.00 37.25
ATOM	2725	CB	MET	537	73.951	11.034	26.549	1.00 46.08
ATOM	2726	CG	MET	537	74.862	12.272	26.619	1.00 57.95
MOTA	2727	SD	MET	537	76.159	12.203	27.919	1.00 66.50
MOTA	2728	CE	MET	537	75.287	12.873	29.377	1.00 64.52
ATOM	2729	С	MET	537	73.749	8.537	26.523	1.00 36.05
ATOM	2730	0	MET	537	74.021	7.865	27.514	1.00 36.71
ATOM	2731	N	ILE	538	72.730	8.255	25.719	1.00 33.77
MOTA	2732	CA	ILE	538	71.804	7.160	26.007	1.00 30.52
MOTA	2733	CB	ILE	538	70.616	7.172	25.012	1.00 28.15
MOTA	2734	CG2	ILE	538	69.780	5.899	25.122	1.00 26.08
MOTA	2735	CG1	ILE	538	69.729	8.377	25.289	1.00 26.24
ATOM	2736	CD1	ILE	538	68.644	8.558	24.256	1.00 26.87
MOTA	2737	С	ILE	538	72.399	5.750	26.100	1.00 30.05
ATOM	2738	0	ILE	538	71.984	4.950	26.941	1.00 31.57
MOTA	2739	N	GLY	539	73.320	5.424	25.211	1.00 30.34
ATOM	2740	CA	GLY	539	73.910	4.103	25.249	1.00 28.22
ATOM	2741	C	GLY	539	73.158	3.094	24.408	1.00 31.25
ATOM	2742	0	GLY	539	72.050	3.359	23.935	1.00 32.88
ATOM	2743	N	LYS	540	73.781	1.933	24.221	1.00 31.96
ATOM	2744	CA	LYS	540	73.222	0.845	23.416	1.00 33.40
ATOM	2745	CB	LYS	540	74.342	-0.023	22.878	1.00 31.53
ATOM	2746	CG	LYS	540	75.177	0.645	21.846	1.00 37.05
ATOM	2747	CD	LYS	540	76.273	-0.266	21.361	1.00 40.15
ATOM	2748	CE	LYS	540	77.143	0.480	20.363	1.00 46.84
ATOM	2749	NZ	LYS	540	76.374	0.920	19.152	1.00 48.60
ATOM	2750	C	LYS	540	72.183	-0.090	24.023	1.00 46.80
	_ , 50	_		5.0	, 2 . 103	0.090	44.023	1.00 30.22

ATO	M 275	:1 6						
ATO			) LY		72.23	7 -0.430	25.215	1.00 40.10
ATO			I HIS		71.254	-0.521		
ATO			A HIS		70.223			
	•		B HIS		69.064			
ATON		_	G HIS		68.127			
ATOM	•		D2 HIS		68.127			
ATOM	- · <del>-</del>		D1 HIS		67.086			
ATOM			E1 HIS		66.489			
ATOM	_		E2 HIS	541	67.096			
ATOM	_	0 C	HIS	541	69.720			1.00 30.46
ATOM		1 0	HIS	541	69.648	-1.614	22.275	1.00 35.33
ATOM	276	2 N	LYS	542	69.348	-3.478	21.200	1.00 34.87
ATOM	276:	3 C2	A LYS		68.908		22.430	1.00 35.42
ATOM		4 CI		542	68.715	-4.311	21.306	1.00 32.02
ATOM	2765	5 C	LYS	542		-5.766	21.753	1.00 30.96
MOTA	2766		LYS	542	67.652	-3.848	20.614	1.00 30.02
ATOM	2767		ASN	543	67.474	-4.058	19.417	1.00 29.10
ATOM	2768			543	66.778	-3.212	21.369	1.00 28.54
ATOM	2769	-			65.529	-2.754	20.803	1.00 28.20
ATOM	2770			543	64.372	-3.241	21.660	1.00 29.73
ATOM	2771		1 ASN	543	64.387	-4.739	21.840	1.00 30.74
ATOM	2772			543	64.732	-5.242	22.909	1.00 32.96
ATOM	2773		2 ASN	543	64.053	-5.462	20.787	1.00 29.58
ATOM	2774		ASN	543	65.426	-1.257	20.529	1.00 28.06
ATOM		_	ASN	543	64.342	-0.679	20.647	1.00 28.86
ATOM	2775		ILE	544	66.546	-0.635	20.168	1.00 26.70
ATOM	2776	CA		544	66.582	0.794	19.833	1.00 26.81
	2777	CB	ILE	544	67.052	1.721	21.019	1.00 24.75
ATOM	2778	CG:		544	66.338	1.353	22.306	1.00 20.02
ATOM	2779	- CG		544	68.568	1.614	21.234	1.00 23.73
ATOM	2780	CD:	l ILE	544	69.105	2.531	22.332	1.00 23.73
ATOM	2781	C	ILE	544	67.582	0.901	18.680	1.00 21.64
ATOM	2782	0	ILE	544	68.388	-0.008	18.480	
ATOM	2783	N	ILE	545	67.449	1.940	17.849	1.00 26.80
ATOM	2784	CA	ILE	545	68.376	2.163	16.745	1.00 29.22
ATOM	2785	CB	ILE	545	67.824	3.164	15.709	1.00 27.14
MOTA	2786	CG2	ILE	545	68.920	3.556	14.731	1.00 26.10
MOTA	2787	CG1	ILE	545	66.625	2.568		1.00 24.70
ATOM	2788	CD1	ILE	545	66.988			1.00 23.78
ATOM	2789	C	ILE	545	69.631			1.00 22.15
ATOM	2790	0	ILE	545	69.586			1.00 28.14
ATOM	2791	N	ASN	546	70.740		18.068	1.00 28.21
ATOM	2792	CA	ASN	546	72.004			1.00 28.40
ATOM	2793	CB	ASN	546		_		1.00 28.49
ATOM	2794	CG	ASN	546	72.709			1.00 27.05
ATOM	2795		ASN	546	71.956		19.470	1.00 27.29
ATOM	2796		ASN		71.793	1.031	20.540	1.00 29.92
ATOM	2797	C		546 546	71.472		19.235	1.00 24.63
ATOM	2798	0	ASN	546	72.982			L.00 28.39
ATOM	2799		ASN	546	73.045	2.894		1.00 29.62
ATOM		N	LEU	547	73.774	3.982		1.00 29.91
ATOM	2800	CA	LEU	547	74.828			1.00 30.68
ATOM	2801	CB	LEU	547	75.297			1.00 25.28
AL ON	2802	CG	LEU	547	76.367			00 24.81
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MOTA	2803	CD1	LEU	547	75.868	7.524	15.990	1.00 22.25
ATOM	2804	CD2	LEU	547	76.716	7.853	18.313	1.00 24.17
ATOM	2805	С	LEU	547	76.016	3.812	16.629	1.00 31.67
ATOM	2806	0	LEU	547	76.481	3.090	17.509	1.00 31.34
ATOM	2807	N	LEU	548	76.475	3.823	15.380	1.00 30.60
ATOM	2808	CA	LEU	548	77.594	2.995	14.955	1.00 29.31
MOTA	2809	CB	LEU	548	77.197	2.165	13.729	1.00 25.94
ATOM	2810	CG	LEU	548	75.968	1.247	13.883	1.00 28.78
MOTA	2811	CD1	LEU	548	75.848	0.360	12.659	1.00 27.14
ATOM	2812	CD2	LEU	548	76.049	0.392	15.149	1.00 23.72
ATOM	2813	С	LEU	548	78.850	3.821	14.644	1.00 31.60
ATOM	2814	0	LEU	548	79.967	3.330	14.753	1.00 32.65
ATOM	2815	N	GLY	549	78.665	5.076	14.248	1.00 32.22
ATOM	2816	CA	GLY	549	79.795	5.928	13.937	1.00 31.40
ATOM	2817	C	GLY	549	79.344	7.267	13.391	1.00 30.78
MOTA	2818	0	GLY	549	78.140	7.536	13.291	1.00 29.84
ATOM	2819	N	ALA	550	80.320	8.099	13.045	1.00 31.88
ATOM	2820	CA	ALA	550	80.073	9.416	12.485	1.00 30.14
ATOM	2821	CB	ALA	550	79.634	10.382	13.590	1.00 31.08
ATOM	2822	С	ALA	550	81.291	9.978	11.742	1.00 28.78
ATOM	2823	0	ALA	550	82.447	9.705	12.102	1.00 26.39
ATOM	2824	N	CYS	551	81.011	10.690	10.651	1.00 28.48
ATOM	2825	CA	CYS	551	82.012	11.391	9.846	1.00 23.69
ATOM	2826	CB	CYS	551	81.825	11.128	8.352	1.00 24.18
ATOM	2827	SG	CYS	551	81.870	9.395	7.840	1.00 28.40
ATOM	2828	C	CYS	551	81.612	12.847	10.127	1.00 20.99
ATOM	2829	0	CYS	551	80.561	13.282	9.684	1.00 22.11
ATOM	2830	N	THR	552	82.357	13.524	10.996	1.00 20.18
ATOM	2831	CA	THR	552	82.073	14.914	11.349	1.00 22.79
ATOM	2832	CB	THR	552	82.090	15.080	12.874	1.00 23.16
ATOM	2833		THR	552	83.408	14.803	13.363	1.00 23.52
ATOM ATOM	2834	CG2 C	THR	552 552	81.125	14.112	13.529	1.00 25.31
ATOM	2835 2836	0	THR THR	552 552	83.138	15.886	10.824	1.00 24.74
ATOM	2837	N	GLN	552	82.939	17.103	10.782	1.00 22.75
ATOM	2838	CA	GLN	553 553	84.276 85.387	15.334	10.431	1.00 26.82
ATOM	2839	CB	GLN	553	86.686	16.153 15.627	9.980	1.00 26.99 1.00 26.40
ATOM	2840	CG	GLN	553	86.632	15.494	10.602 12.141	1.00 28.40
ATOM	2841	CD	GLN	553	86.438	16.836	12.141	1.00 22.89
ATOM	2842		GLN	553	87.259	17.729	12.656	1.00 25.90
ATOM	2843		GLN	553	85.351	16.994	13.566	1.00 23.53
ATOM	2844	С	GLN	553	85.502	16.216	8.466	1.00 25.33
ATOM	2845	Ō	GLN	553	85.177	15.259	7.779	1.00 20.23
ATOM	2846	N	ASP	554	85.863	17.394	7.968	1.00 30.00
ATOM	2847	CA	ASP	554	86.084	17.631	6.531	1.00 28.38
ATOM	2848	CB	ASP	554	87.410	17.031	6.105	1.00 26.38
ATOM	2849	CG	ASP	554	88.538	17.570	6.912	1.00 28.78
ATOM	2850	OD1		554	88.789	18.795	6.823	1.00 31.33
ATOM	2851	OD2		554	89.141	16.795	7.665	1.00 35.18
ATOM	2852	C	ASP	554	85.011	17.221	5.545	1.00 29.04
ATOM	2853	0	ASP	554	85.278	16.468	4.610	1.00 23.14
ATOM	2854	N	GLY	555	83.824	17.793	5.709	1.00 31.22
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ATO		55	CA GL	Y 555	82.72	3 17 40	0 4 55	
ATO		56	C GL	Y 555	81.446			
ATON		57 (	O GL		81.448			2 21.04
ATON	1 28	58 J	N PR		80.317			
ATOM		59 (	CD PR		80.213			,
ATOM	1 28	50 (	CA PRO					
ATOM	1 286	51 (	CB PRO		79.010			
ATOM	1 286		G PRO		78.107			1.00 22.88
ATOM	286				79.077	-		1.00 23.50
ATOM					79.006			1.00 27.67
ATOM					79.676			1.00 27.13
ATOM		_	A LEU		78.253			1.00 29.27
ATOM			B LEU		78.164	15.405		1.00 31.19
ATOM					77.583	16.130		1.00 29.94
ATOM			D1 LEU		77.019	15.260		1.00 26.87
ATOM	287		D2 LEU		78.131	14.540	12.062	1.00 23.83
ATOM	287				76.237	16.146	12.275	1.00 23.80
ATOM	287		LEU		77.291	14.193	8.651	1.00 31.97
ATOM	287	_	LEU		76.158	14.332	8.184	1.00 31.18
ATOM	2874		TYR		77.857	13.010	8.882	1.00 31.12
ATOM	2879				77.145	11.767	8.664	1.00 28.86
ATOM	2876			558	77.905	10.869	7.694	1.00 28.58
ATOM	2877			558	78.017	11.395	6.281	1.00 32.33
ATOM	2878		1 TYR	558	79.034	10.962	5.443	1.00 35.23
ATOM	2879		I TYR	558	79.161	11.447	4.151	1.00 37.54
ATOM			2 TYR	558	77.123	12.336	5.787	1.00 35.27
ATOM	2880			558	77.248	12.832	4.493	1.00 36.43
ATOM	2881			558	78.276	12.382	3.680	1.00 37.05
ATOM	2882			558	78.423	12.869	2.394	1.00 39.97
ATOM	2883		TYR	558	77.000	11.071	10.004	1.00 26.63
ATOM	2884	_	TYR	558	77.985	10.885	10.725	1.00 24.67
ATOM	2885		VAL	559	75.756	10.774	10.365	1.00 28.15
ATOM	2886	CA		559	75.429	10.070	11.610	1.00 27.70
ATOM	2887	CB	VAL	559	74.262	10.770	12.372	1.00 26.63
ATOM	2888		l VAL	559	73.876	9.959	13.603	1.00 24.70
ATOM	2889	CG2		559	74.673	12.186		1.00 24.70
ATOM	2890	С	VAL	559	75.061	8.635		1.00 25.71
ATOM	2891	0	VAL	559	73.965	8.357		1.00 27.08
ATOM	2892 2893	N	ILE	560	76.002	7.729		1.00 28.25
ATOM		CA	ILE	560	75.820	6.335	7.7 000	1.00 29.62
ATOM	2894	CB	ILE	560	77.225			1.00 30.06
ATOM	2895		ILE	560	77.045			1.00 30.06
	2896		ILE	560	78.004	6.557		1.00 31.58
ATOM	2897	CD1	ILE	560	79.492	6.239	9.629	27.50
ATOM	2898	С	ILE	560	75.075			1.00 23.31
ATOM	2899	0	ILE	560	75.586			1.00 29.88
ATOM	2900	N	VAL	561	73.857		11 607 3	.00 27.32
ATOM	2901	CA	VAL	561	73.053			00 29.09
ATOM	2902	CB	VAL	561	71.743			.00 28.70
ATOM	2903		VAL	561	72.072			.00 25.29
MOTA	2904	CG2	VAL	561	70.887			.00 22.91
ATOM	2905	С	VAL	561	72.731			.00 22.38
ATOM	2906	0	VAL	561			1.945 1	.00 27.99
				_	. 5 . 652	2.590 1	.0.783 1	.00 27.88

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ATOM	2907	N	GLU	562	72.143	1.969	12.754	1.00 27.38
ATOM	2908	CA	GLU	562	71. <b>75</b> 9	0.616	12.347	1.00 28.01
MOTA	2909	CB	GLU	562	71.246	-0.161	13.555	1.00 25.37
ATOM	2910	CG	GLU	562	72.322	-0.487	14.570	1.00 29.22
MOTA	2911	CD	GLU	562	71.785	1.190	15.796	1.00 30.94
MOTA	2912	OE1	GLU	562	72.440	-2.135	16.271	1.00 34.82
ATOM	2913	OE2	GLU	562	70.716	-0.795	16.297	1.00 32.77
MOTA	2914	C	GLU	562	70.695	0.610	11.266	1.00 29.83
MOTA	2915	0	GLU	562	69.822	1.452	11.274	1.00 34.69
MOTA	2916	N	TYR	563	70.755	-0.364	10.362	1.00 31.35
MOTA	2917	CA	TYR	563	69.806	-0.527	9.255	1.00 33.79
MOTA	2918	CB	TYR	563	70.586	-0.987	8.022	1.00 32.37
ATOM	2919	CG	TYR	563	69.759	-1.232	6.778	1.00 31.70
ATOM	2920	CD1	TYR	563	68.858	-0.277	6.319	1.00 35.00
MOTA	2921	CE1	TYR	563	68.101	-0.490	5.161	1.00 35.62
ATOM	2922	CD2	TYR	563	69.888	-2.416	6.053	1.00 31.64
MOTA	2923	CE2	TYR	563	69.138	-2.644	4.894	1.00 32.96
MOTA	2924	CZ	TYR	563	68.242	-1.674	4.462	1.00 36.20
ATOM	2925	OH	TYR	563	67.494	-1.906	3.340	1.00 39.54
ATOM	2926	С	TYR	563	68.668	-1.527	9.593	1.00 37.26
ATOM	2927	0	TYR	563	68.915	-2.566	10.212	1.00 38.86
ATOM	2928	N	ALA	564	67.428	-1.180	9.220	1.00 39.09
MOTA	2929	CA	ALA	564	66.256		9.467	1.00 37.64
ATOM	2930	CB	ALA	564	65.290	-1.317	10.366	1.00 41.34
ATOM	2931	C	ALA	564	65.600	-2.337	8.124	1.00 39.33
ATOM	2932	0	ALA	564	64.700	-1.628	7.661	1.00 41.28
MOTA	2933	N	SER	565	66.033	-3.432	7.515	1.00 40.21
MOTA	2934	CA	SER	565	65.567	-3.867	6.202	1.00 40.22
MOTA	2935	CB	SER	565	66.302	-5.133	5.808	1.00 38.50
ATOM	2936	OG	SER	565	66.174	-6.084	6.847	1.00 37.66
ATOM	2937	C	SER	565	64.095	-4.087	5.987	1.00 42.30
ATOM	2938	0	SER	565	63.657	-4.155	4.840	1.00 46.83
ATOM	2939	N	LYS	566	63.322	-4.248	7.054	1.00 42.84
MOTA	2940	CA	LYS	566	61.893	-4.462	6.883	1.00 41.84
MOTA	2941	CB	LYS	566	61.455	-5.681	7.684	1.00 44.88
MOTA	2942	CG	LYS	566	62.003	-6.977	7.088	1.00 48.86
ATOM	2943	CD	LYS	566	61.929	-8.148	8.040	1.00 51.41
MOTA	2944	CE	LYS	566	62.582	-9.362	7.426	1.00 53.89
ATOM	2945	NZ	LYS	566		-10.465	8.417	1.00 59.37
ATOM	2946	С	LYS	566	61.029	-3.234	7.143	1.00 41.89
ATOM	2947	0	LYS	566	59.815	-3.337	7.341	1.00 43.68
ATOM	2948	N	GLY	567	61.663	-2.061	7.100	1.00 39.50
ATOM	2949	CA	GLY	567	60.956	-0.808	7.291	1.00 36.69
ATOM	2950	C	GLY	567	60.306	-0.640	8.644	1.00 35.86
ATOM	2951	0	GLY	567	60.727	-1.265	9.614	1.00 35.90
ATOM	2952	N	ASN	568	59.296	0.218	8.711	1.00 35.45
ATOM	2953	CA	ASN	568	58.615	0.447	9.966	1.00 38.10
ATOM	2954	CB	ASN	568	57.961	1.839	10.029	1.00 40.77
ATOM	2955	CG	ASN	568	56.701	1.962	9.163	1.00 43.52
ATOM	2956	OD1		568	55.718	1.241	9.338	1.00 44.01
ATOM	2957	ND2		568	56.710	2.932	8.263	1.00 45.39
ATOM	2958	С	ASN	568	57.610	-0.657	10.269	1.00 38.91

ATO	M 20		_					
ATO			O AS		57.2	18 -1.420	9.384	1 1.00 39.95
			N LE		57.20			33.33
ATO			CA LE	U 569	56.25			
ATO			CB LE	U 569	56.12			
ATO			CG LE		55.15			
ATO			CD1 LE		55.55			
ATOM		65 (	CD2 LET	J 569	55.14			
ATOM		66 (	LE		54.87		- <del>-</del>	
ATOM	1 296	57 (	LE		54.23		<del>-</del>	
ATOM	1 296	8 8			54.38	_		
ATOM	1 29€	9 0	A ARG		53.06			1.00 36.63
ATOM	297	0 C	B ARG			_		1.00 36.68
ATOM	297	'1 C	G ARG		52.73	_	10.188	1.00 37.76
ATOM	297		D ARG		51.33	_	9.623	1.00 46.41
ATOM		-			51.21		8.889	1.00 56.33
ATOM				- · •	52.162		7.779	1.00 63.05
ATOM		_	E ARG		53.010		7.603	1.00 66.33
ATOM					53.032		8.468	1.00 65.15
ATOM			H2 ARG		53.853		6.580	1.00 66.56
ATOM	297	_	ARG	•	53.046		9.193	1.00 35.55
ATOM			ARG		52.248	-2.015	9.018	1.00 35.33
ATOM	297		GLU	571	53.978	-0.758	8.320	1.00 37.20
ATOM	2980			571	54.128	-1.401	7.030	1.00 38.32
ATOM	2983			5 <b>7</b> 1	55.247	-0.695	6.261	1.00 40.15
	2982			571	55.001		6.152	
ATOM	2983			571	56.118	1.557	5.442	1.00 49.09
ATOM	2984		1 GLU	571	57.279	1.073	5.421	1.00 58.16
MOTA	2985	-	2 GLU	571	55.824	2.660	4.914	1.00 61.41
ATOM	2986	-	GLU	571	54.406	-2.906		1.00 61.27
ATOM	2987		GLU	571	53.863	-3.721	7.170	1.00 36.74
ATOM	2988	N	TYR	572	55.241	-3.266	6.410	1.00 35.74
ATOM	2989	CA	TYR	572	55.591	-4.665	8.141	1.00 35.13
ATOM	2990	CB	TYR	572	56.591	-4.736	8.401	1.00 37.12
ATOM	2991	CG	TYR	572	56.984		9.560	1.00 34.39
MOTA	2992	CD	1 TYR	572	57.980	-6.128	10.029	1.00 33.48
ATOM	2993	CE:		572	58.394	-6.869	9.367	1.00 29.76
MOTA	2994	CD:	2 TYR	572	56.406	-8.119		1.00 27.14
ATOM	2995	CE:		572	56.814	-6.681		1.00 32.40
MOTA	2996	CZ	TYR	572	57.807			1.00 30.83
MOTA	2997	ОН	TYR	572	58.201			1.00 33.73
MOTA	2998	C	TYR	572				1.00 37.16
ATOM	2999	0	TYR	572	54.330	-5.468		1.00 38.92
ATOM	3000	N	LEU	573	54.108	-6.553	8.183	1.00 39.22
ATOM	3001	CA	LEU		53.507	-4.922	9.618	1.00 38.41
ATOM	3002	СВ	LEU	573	52.261	-5.563	10.016	L.00 37.56
ATOM	3003	CG	LEU	573	51.573	-4.711	11.084	L.00 36.44
ATOM	3004		LEU	573	52.270	-4.617	12.437	1.00 33.91
ATOM	3005		LEU	573 573	51.555	-3.626		.00 31.60
ATOM	3006	CD2		573	52.313	-6.024		00 30.78
ATOM	3007		LEU	573	51.315	~5.738		00 37.51
ATOM		0	LEU	573	50.847	-6.836		.00 36.70
ATOM	3008	И	GLN	574	51.045	-4.643		.00 40.10
ATOM	3009	CA	GLN	574	50.141	-4.678		.00 41.10
AIOM	3010	CB	GLN	574	49.938			.00 40.12
		-					1	.00 40.12

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ATOM	3011	CG	GLN	574	49.171	-2.381	7.374	1.00	40.77
MOTA	3012	CD	GLN	574	49.079	-0.987	6.852	1.00	43.90
ATOM	3013	OE1	GLN	574	49.679	-0.652	5.835	1.00	46.93
MOTA	3014	NE2	GLN	574	48.357	-0.143	7.558	1.00	46.85
MOTA	3015	C	GLN	574	50.546	-5.638	5.875	1.00	41.31
ATOM	3016	0	GLN	574	49.699	-6.323	5.309	1.00	44.33
ATOM	3017	N	ALA	575	51.840	-5.735	5.601	1.00	41.46
ATOM	3018	CA	ALA	575	52.317	-6.628	4.555	1.00	39.80
ATOM	3019	CB	ALA	575	53.745	-6.301	4.218	1.00	40.58
MOTA	3020	С	ALA	575	52.197	-8.096	4.947	1.00	40.86
ATOM	3021	0	ALA	575	52.527	-8.975	4.165	1.00	41.50
ATOM	3022	N	ARG	576	51.757	-8.359	6.168	1.00	42.47
ATOM	3023	CA	ARG	576	51.624	-9.726	6.641	1.00	42.68
ATOM	3024	CB	ARG	576	52.679	-9.988	7.716	1.00	41.04
MOTA	3025	CG	ARG	576	54.095	-9.958	7.161	1.00	42.73
ATOM	3026	CD	ARG	576	55.156	-9.943	8.257	1.00	45.59
ATOM	3027	NE	ARG	576	56.514	-9.870	7.695	1.00	43.89
ATOM	3028	CZ	ARG	576	56.981	-8.856	6.969	1.00	43.35
ATOM	3029		ARG	576	56.219	-7.803	6.703	1.00	44.85
ATOM	3030		ARG	576	58.215	-8.902	6.497	1.00	41.84
MOTA	3031	C	ARG	576	50.232	-10.014	7.180	1.00	44.86
MOTA	3032	0	ARG	576	50.043	-10.943	7.970	1.00	46.08
MOTA	3033	N	ARG	577	49.258	-9.216	6.753	1.00	46.72
MOTA	3034	C,Y	ARG	577	47.877	-9.401	7.196	1.00	47.61
ATOM	3035	CB	ARG	577	46.994	-8.239	6.723		46.35
ATOM	3036	CG	ARG	577	47.101	-6.995	7.581	1.00	47.71
ATOM	3037	CD	ARG	577	46.329	-5.831	6.999		49.15
ATOM	3038	NE	ARG	577	46.213	-4.735	7.957	1.00	53.23
ATOM	3039	CZ	ARG	577	45.584	-3.587	7.725		54.38
ATOM	3040	NH1		577 .	45.020	-3.368	6.549		56.41
ATOM	3041	NH2		577	45.481	-2.676	8.686		58.13
ATOM	3042	С	ARG	577		-10.740	6.743		47.36
ATOM	3043	0	ARG	577		-11.031	5.550		48.52
MOTA	3044	N	GLN	594		-13.948	7.960		68.05
MOTA	3045	CA	GLN	594		-14.067	8.772		66.75
ATOM ATOM	3046	CB	GLN	594		-15.220	8.277		66.87
ATOM	3047 3048	C	GLN	594		-14.284	10.233		64.71
ATOM	3048	И	GLN LEU	594		-15.264	10.580		64.86
ATOM	3049	CA		595		-13.335	11.074		61.14
ATOM	3050	CB	LEU	595 595		-13.422	12.480	1.00	
ATOM	3052	CG	LEU LEU	395 505		-12.008	13.056	1.00	
ATOM	3052	CD1		595 595		-11.147	12.203	1.00	
ATOM	3054	CD2		595	53.375	-9.692	12.533	1.00	
ATOM	3055	C	LEU	595		-11.598	12.382	1.00	
ATOM	3056	0	LEU			-14.237	13.251	1.00	
ATOM	3057	N	SER	595 <b>59</b> 6		-14.359 -14.845	12.834	1.00	
ATOM	3058	CA	SER	596			14.341	1.00	
ATOM	3059	CB	SER	596		-15.642	15.229	1.00	
ATOM	3060	OG	SER	596		-16.841 -16.435	15.736	1.00	
ATOM	3061	C	SER	596		-16.435 -14.756	16.737	1.00	
ATOM	3062	0	SER	596		-14.756 -13.767	16.423	1.00	
	3002	•	JEK	J 7 U	J1.474	-13.707	16.649	1.00	47.39

ATC		063	N S	SER 59	7 49.833 -15.163 17.242 1 00 50 27
ATO		64	CA S	ER 59	7 49 469 34 305
ATO		65		ER 59	7 48 301 15 15 1
ATO		66	OG S	ER 59	7 47 540 35 05
ATO		67	C S	ER 59	7 50 605 14 145
ATO			0 s	ER 59	7 50 792 12 222
ATO			N L	YS 598	51 612 15 100
ATO			CA L	YS 598	52 824 - 14 05
ATON				YS 598	53 566 176 205 - 1.00 53.84
ATON			CG L	YS 598	54 376 36 457
ATOM ATOM			CD L	(S 598	55 057 17 00
ATOM			CE L'		55 700 70 000
ATOM		_	NZ LY		54 840 -10 160 - 1.00 39.00
ATOM			C LY		53 720 12 000
ATOM		_	D L'A	•	54 272 12 252
ATOM					53 842 -13 000 2.00 51.72
ATOM			CA AS		54.657 -13 001 15
ATOM			B AS		54 569 13 20
ATOM	308 308	-	G As		55 222 14 50-
ATOM	308	_	D1 AS		55.898 -15 260 26 26
ATOM	3084		D2 AS	_	55 100 14 000
ATOM	3085	_			54 173 -11 500
ATOM	3086				54.976 -10.703 17.960 1.00 52.06
ATOM	3087				52.852 -11.406 17.684 1.00 44.53
ATOM	3088				52.272 -10.099 17.938 1 00 41 05
ATOM	3089				50.774 -10.100 17.632 1 00 30 33
ATOM	3090		ol LEC		50.354 -10.374 16.178 1 00 36 50
ATOM	3091		2 LEU		48.850 -10.272 16.063 1 00 34 00
ATOM	3092		LEU		51.000 -9.393 15.232 1.00 33 72
ATOM	3093		LEU	600 600	52.543 -9.633 19.369 1.00 40 96
MOTA	3094	N	VAL	601	32.830 ~8.467 19.580 7.00 42.04
ATOM	3095	CA		601	32.41/-10.533 20.348 1 00 41 02
ATOM	3096	CB		601	52.005 -10.156 21.744 1.00 43.57
ATOM	3097		1 VAL	601	32.236 -11.229 22.791 1 00 43 60
ATOM	3098		2 VAL	601	52.254 -10.607 24.205 1.00 43.44
ATOM	3099	C	VAL	601	50.848 -11.761 22.464 1.00 42.33
MOTA	3100	0	VAL	601	54.611 2 21.901 1.00 42.85
ATOM	3101	N	SER	602	54 996 70 60-
ATOM	3102	CA	SER	602	54.986 -10.685 21.175 1.00 41.33 56.442 -10.581 21.180 1.00 41.43
ATOM	3103	CB	SER	602	E7 014
ATOM	3104	OG	SER	602	50 424 22 65
ATOM	3105	С	SER	602	EC 050
ATOM	3106	0	SER	602	E7 C20 - 1.00 40.58
ATOM	3107	N	CYS	603	56 370 2 32.403 1.00 42.32
ATOM	3108	CA	CYS	603	56 500 7 100 38.34
ATOM	3109	CB	CYS	603	EE 715 5 1.00 37.28
ATOM	3110	SG	CYS	603	55 735 5 1.00 38.09
ATOM	3111	С	CYS	603	56 202 6 227
ATOM	3112	0	CYS	603	57 030 5 000 100 35.81
ATOM	3113	N	ALA	604	55 199 6 500
ATOM	3114	CA	ALA	604	54 904 5
					34.804 -5.572 21.911 1.00 34.97

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ATOM	3115	CB	ALA	604	53.393	-5.917	22.409	1.00 34.13
ATOM	3116	С	ALA	604	55.791	-5.610	23.081	1.00 36.68
MOTA	3117	0	ALA	604	56.085	-4.585	23.704	1.00 36.78
ATOM	3118	N	TYR	605	56.281	-6.807	23.385	1.00 37.68
ATOM	3119	CA	TYR	605	57.254	-7.005	24.461	1.00 38.38
ATOM	3120	CB	TYR	605	57.533	-8.498	24.643	1.00 37.62
ATOM	3121	CG	TYR	605	58.635	-8.806	25.622	1.00 36.56
MOTA	3122	CD1	TYR	605	58.498	-8.509	26.974	1.00 39.05
MOTA	3123	CE1	TYR	605	59.520	-8.809	27.893	1.00 41.37
MOTA	3124	CD2	TYR	605	59.812	-9.407	25.198	1.00 38.09
MOTA	3125	CE2	TYR	605	60.848	-9.711	26.105	1.00 38.55
ATOM	3126	CZ	TYR	605	60.692	-9.409	27.454	1.00 40.73
MOTA	3127	OH	TYR	605	61.707	-9.704	28.348	1.00 41.44
ATOM	3128	C	TYR	605	58.549	-6.267	24.123	1.00 38.44
ATOM	3129	0	TYR	605	59.053	-5.485	24.937	1.00 40.78
ATOM	3130	N	GLN	606	59.053	-6.501	22.908	1.00 36.07
ATOM	3131	CA	GLN	606	60.276	-5.872	22.398	1.00 35.28
ATOM	3132	CB	GLN	606	60.594	-6.415	21.002	1.00 34.24
ATOM	3133	CG	GLN	606	61.105	-7.851	21.005	1.00 32.26
ATOM	3134	CD	GLN	606	61.339	-8.388	19.608	1.00 30.17
ATOM	3135	OE1	GLN	606	62.274	-7.988	18.907	1.00 31.89
ATOM	3136	NE2	GLN	606	60.471	-9.285	19.182	1.00 30.68
MOTA	3137	С	GLN	606	60.210	-4.335	22.355	1.00 36.39
MOTA	3138	0	GLN	606	61.206	-3.660	22.632	1.00 39.59
MOTA	3139	N	VAL	607	59.040	-3.798	22.006	1.00 32.78
MOTA	3140	CA	VAL	607	58.839	-2.350	21.944	1.00 30.29
MOTA	3141	CB	VAL	607	57.489	-1.982	21.221	1.00 28.48
ATOM	3142		VAL	607	57.219	-0.488	21.298	1.00 28.68
ATOM	3143		VAL	607	57.535	-2.416	19.742	1.00 22.96
ATOM	3144	С	VAL	607	58.868	-1.766	23.364	1.00 30.21
ATOM	3145	0	VAL	607	59.469	-0.705	23.591	1.00 31.24
ATOM	3146	N	ALA	608	58.224	-2.451	24.311	1.00 27.88
ATOM	3147	CA	ALA	608	58.187	-2.001	25.694	1.00 27.66
ATOM	3148	CB	ALA	608	57.242	-2.874	26.494	1.00 26.42
	3149	C	ALA	608	59. <b>5</b> 85	-2.019	26.309	1.00 29.04
ATOM	3150	0	ALA	608	59.950	-1.144	27.094	1.00 27.53
ATOM	3151	N	ARG	609	60.377	-3.013	25.932	1.00 28.91
ATOM	3152	CA	ARG	609	61.733	-3.120	26.440	1.00 31.64
ATOM	3153	CB	ARG	609	62.394	-4.405	25.953	1.00 33.78
ATOM	3154	CG	ARG	609	61.672	-5.647	26.373	1.00 38.53
ATOM	3155	CD	ARG	609	62.636	-6.791	26.448	1.00 41.78
ATOM	3156	NE	ARG	609	63.319	-6.838	27.733	1.00 47.58
ATOM	3157	CZ	ARG	609	64.441	-7.510	27.955	1.00 51.52
MOTA	3158		ARG	609	65.012	-8.179	26.964	1.00 50.61
MOTA	3159		ARG	609	64.954	-7.569	29.186	1.00 54.36
MOTA	3160	C	ARG	609	62.581	-1.918	26.024	1.00 33.26
ATOM	3161	0	ARG	609	63.144	-1.221	26.885	1.00 34.50
ATOM	3162	N	GLY	610	62.624	-1.650	24.717	1.00 30.25
ATOM	3163	CA	GLY	610	63.395	-0.534	24.199	1.00 25.40
ATOM	3164	C	GLY	610	63.010	0.730	24.930	1.00 24.12
ATOM	3165	0	GLY	610	63.857	1.507	25.345	1.00 24.74
ATOM	3166	N	MET	611	61.712	0.907	25.131	1.00 25.81



AT	OM -										
		167		MET	611	61.19	92 2 (	062 25.			
ATC ATC	-	168	CB	MET	611	59.67					26.95
	·-·	169	CG	MET	611	59.21					24.60
ATO		170	SD	MET	611	59.97				.00 2	24.10
ATC		171		MET	611	59.54				.00 2	26. <b>7</b> 7
ATC		172	C I	MET	611	61.60				.00 1	19.21
ATO		173	0 1	/ET	611	61.89					7.68
ATO		74	N (	LU	612	61.56	_			.00 2	8.22
ATO		.75	CA C	LU	612	61.95				. 00 з	1.07
ATO		76	CB G	LU	612	61.80			82 1.	00 3	
ATO		77	CG G	LU	612	62.38			72 1.	00 3	
ATO		78		LU	612				571.	00 3	
ATO			OE1 G	LU	612	62.392			31 1.	00 3	
ATOM		80	OE2 G	LU	612	62.599			38 1.	00 3	0.09
ATON	1 31:			LՄ	612	62.226	-			00 33	
ATOM	1 31		_	LԾ	612	63.409		29.46		00 37	
ATOM		33 <u>1</u>		YR	613	63.791		5 30.39	0 1.	00 35	60
ATOM				rR	613	64.196		8 28.45		00 37	
ATOM	318			/R	613	65.601		7 28.39		00 36	. 60
ATOM	318		G TY			66.328			6 1.0	00 34	23
ATOM	318		DI TY		613	67.801	_		5 1.0	00 36	50
ATOM	318		El TY		613	68.734	0.26	3 28.00		00 36	
MOTA			D2 TY		613	70.090	0.64	9 28.01		0 34	51
ATOM		_	E2 TY		613	68.252	1.909	9 26.33		0 35	
ATOM	319				613	69.596	2.306	26.34		0 34	
ATOM	319	_			613	70.512	1.674	27.18		0 35	.09
ATOM	319				613	71.826	2.089	27.212		0 29	. 91
ATOM	319				613	65.724	2.760			0 37.	. /8
ATOM	319	_			613	66.362	3.414	29.056		0 37.	
ATOM	3196		LEI		614	65.081	3.326		-	0 35.	
ATOM	3197				614	65.156	4.766	26.988		0 34.	
ATOM	3198				614	64.314	5.157			31.	
ATOM	3199		LEC LEC		614	64.760	4.601	24.429		29.	68
ATOM	3200				614	63.783	5.016	23.346		29.	
ATOM	3201				614	66.134	5.133	24.111		32.	
ATOM	3202	_	LEU		614	64.698	5.538	28.218		36.	
ATOM	3202		LEU		514	65.325	6.525	28.618			
ATOM	3204		ALA		515	63.608	5.076	28.821	1.00	33.1 38.6	8.T
ATOM	3205				515	63.066	5.711	30.018	1.00	41.0	28
ATOM	3206				515	61.767	5.018	30.444			
ATOM	3207	~	ALA		515	64.099	5.683	31.147	1.00	42.3	33
ATOM	3207	0	ALA		15	64.291	6.690	31.831		40.4	
ATOM		N	SER		16	64.788	4.553	31.307		41.2	
ATOM	3209	CA	SER	6	16	65.806	4.441	32.347	1.00	38.7	'8
ATOM	3210	CB	SER	6	16	66.354	3.009	32.454	1.00	40.9	7
ATOM	3211	OG	SER	6	16	67.172	2.651		1.00	37.B	2
ATOM	3212	C	SER	6	16	66.941	5.416	31.359 32.061	1.00	34.7	3
	3213	0	SER	6	16	67.714	5.769		1.00	42.6	8
ATOM	3214	N	LYS	6	17	67.015	5.869	32.957	1.00		
ATOM	3215	CA	LYS		17	68.025	6.816	30.815	1.00		
ATOM	3216	CB	LYS		17	68.541	6.411	30.380	1.00		
ATOM	3217	CG	LYS		17	69.293		29.003	1.00		
ATOM	3218	CD	LYS		L 7	70.421	5.111	29.021	1.00	36.40	)
							5.221	29.992	1.00	38.14	1

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ATOM	3219	CE	LYS	617	71.215	3.941	30.086	1.00	38.43
MOTA	3220	NZ	LYS	617	72.530	4.210	30.751	1.00	43.07
ATOM	3221	С	LYS	617	67.475	8.242	30.350	1.00	38.42
ATOM	3222	0	LYS	617	68.072	9.133	29.744	1.00	41.37
ATOM	3223	N	LYS	618	66.323	8.444	30.985	1.00	37.25
ATOM	3224	CA	LYS	618	65.674	9.743	31.067		36.75
ATOM	3225	CB	LYS	618	66.653	10.780	31.632		43.27
ATOM	3226	CG	LYS	618	67.340	10.392	32.938		51.59
MOTA	3227	CD	LYS	618	66.377	10.361	34.092	1.00	61.24
ATOM	3228	CE	LYS	618	67.070	9.945	35.373		67.83
ATOM	3229	NZ	LYS	618	66.105	10.039	36.510		75.22
MOTA	3230	С	LYS	618	65.167	10.222	29.706	1.00	36.61
MOTA	3231	0	LYS	618	64.856	11.396	29.535		35.94
ATOM	3232	N	CYS	619	65.058	9.308	28.751		36.26
ATOM	3233	CA	CYS	619	64.603	9.666	27.412		33.41
ATOM	3234	CB	CYS	619	65.351	8.843	26.365		32.17
ATOM	3235	SG	CYS	619	65.006	9.223	24.650		26.92
MOTA	3236	С	CYS	619	63.108	9.546	27.194	1.00	32.29
ATOM	3237	0	CYS	619	62.510	8.472	27.373	1.00	29.13
MOTA	3238	N	ILE	620	62.515	10.679	26.827	1.00	31.60
ATOM	3239	CA	ILE	620	61.091	10.763	26.528	1.00	31.21
ATOM	3240	CB	ILE	620	60.435	11.966	27.212	1.00	29.57
ATOM	3241	CG2	ILE	620	58.955	12.031	26.860	1.00	31.49
ATOM	3242	CG1	ILE	620	60.578	11.848	28.727		27.85
ATOM	3243	CD1	ILE	620	60.065	13.046	29.463	1.00	26.50
MOTA	3244	С	ILE	620	61.034	10.972	25.018		32.18
ATOM	3245	0	ILE	620	61.481	11.993	24.512	1.00	33.18
MOTA	3246	N	HIS	621	60.472	9.990	24.318	1.00	31.93
MOTA	3247	CA	HIS	621	60.354	9.970	22.864	1.00	32.59
ATOM	3248	CB	HIS	621	59.933	8.552	22.420	1.00	29.51
MOTA	3249	CG	HIS	621	60.076	8.288	20.951	1.00	27.45
MOTA	3250	CD2	HIS	621	60.663	7.262	20.286	1.00	25.84
MOTA	3251	ND1	HIS	621	59.528	9.106	19.979	1.00	25.20
ATOM	3252	CE1	HIS	621	59.774	8.596	18.783	1.00	25.07
MOTA	3253	NE2	HIS	621	60.456	7.473	18.942	1.00	23.24
ATOM	3254	C	HIS	621	59.365	10.992	22.320	1.00	35.31
MOTA	3255	0	HIS	621	59.555	11.481	21.220	1.00	39.24
ATOM	3256	N	ARG	622	58.256	11.216	23.028		36.50
ATOM	3257	CA	ARG	622	57.225	12.169	22.580	1.00	35.78
MOTA	3258	CB	ARG	622	57.783	13.582	22.462	1.00	32.55
ATOM	3259	CG	ARG	622	58.211	14.156	23.778	1.00	30.54
MOTA	3260	CD	ARG	622	58.799	15.551	23.635	0.50	27.28
ATOM	3261	NE	ARG	622	59.249	16.043	24.930	0.50	24.53
MOTA	3262	CZ	ARG	622	60.409	15.707	25.499	0.50	27.85
MOTA	3263	NHl	ARG	622	61.249	14.883	24.877	0.50	27.61
ATOM	3264	NH2	ARG	622	60.711	16.158	26.714	0.50	25.34
ATOM	3265	C	ARG	622	56.447	11.806	21.297	1.00	35.76
MOTA	3266	0	ARG	622	55.438	12.430	20.999	1.00	36.61
ATOM	3267	N	ASP	623	56.923	10.818	20.537	1.00	34.69
MOTA	3268	CA	ASP	623	56.197	10.400	19.335	1.00	34.09
MOTA	3269	CB	ASP	623	56.628	11.171	18.081	1.00	34.77
ATOM	3270	CG	ASP	623	55.727	10.869	16.863	1.00	43.51



) To									
ATO			OD1 AS			56.21	3 10.99	92 15.71	A 1 00 45 45
ATO			DD2 ASI			54.53		_	
ATO		_	C ASI	623		56.32			
ATO		`	) ASI			56.63			
ATON		_	1 LEU	624		56.083			
ATON			CA LEU	624		56.152			
ATON			B LEU	624		56.133			
ATOM			G LEU	624		55.983			
ATOM			DI LEU			57.108			
ATOM		80 C	D2 LEU	624		56.001			
ATOM		1 0	LEU	624		54.954			,00
ATOM		2 0	LEU			53.805			
ATOM		3 N	ALA			55.224		• • •	
ATOM		4 C	A ALA	625		54.170			· · · · · ·
ATOM		5 C		625		53.707			
ATOM		6 C	ALA	625		54.800			,
ATOM	328	7 0	ALA	625		56.022			
ATOM	328	8 N	ALA	626					
ATOM	328	9 C		626		53.982	3.107		1.00 29.46
ATOM	329	O CE		626		54.499	1.993		1.00 28.16
ATOM	329	L C	ALA	626		53.350			1.00 28.02
ATOM	3292	2 0	ALA	626		55.366	2.504		1.00 26.78
ATOM	3293		ARG	627		56.329	1.859		1.00 26.69
ATOM	3294	CA		627		55.022	3.680		1.00 26.09
ATOM	3295			627		55.777	4.301	12.246	1.00 26.78
ATOM	3296			627		55.134	5.637		1.00 27.01
ATOM	3297					55.046	6.672	12.961	1.00 29.34
ATOM	3298			627 627		54.552	8.037	12.477	1.00 34.26
ATOM	3299					54.108	8.878	13.590	1.00 36.96
ATOM:	3300		1 ARG	627 627		52.867	8.889	14.059	1.00 40.84
ATOM	3301			627		51.942	8.114	13.515	1.00 42.56
ATOM	3302		ARG			52.552	9.634	15.108	1.00 45.20
ATOM	3303	ō	ARG	627		7.209	4.549	12.711	1.00 29.11
ATOM	3304	N	ASN	627		8.137	4.468	11.911	1.00 30.39
ATOM	3305	CA		628		7.385	4.804	14.010	1.00 30.37
ATOM	3306	CB	asn Asn	628		8.689	5.092	14.596	1.00 27.02
ATOM	3307	CG		628		8.578	6.226	15.611	1.00 24.35
ATOM	3308		ASN ASN	628		8.383	7.571	14.941	1.00 25.95
ATOM	3309		ASN ASN	628		8.992	7.865	13.924	1.00 32.01
ATOM	3310	C		628		7.522	8.391	15.503	1.00 24.34
ATOM	3311	0	ASN	628		9.437	3.903	15.185	1.00 26.74
ATOM	3312	N	ASN	628		0.378	4.062	15.972	1.00 28.49
ATOM	3313		VAL	629		8.998	2.712	14.802	1.00 27.34
ATOM	3314	CA	VAL	629	5:	9.621	1.450	15.224	1.00 24.94
ATOM	3314	CB	VAL	629		8.589	0.522	15.906	1.00 22.20
ATOM			VAL	629		9.169	-0.883		1.00 18.03
ATOM	3316		VAL	629		3.158	1.121	_	1.00 18.34
ATOM	3317	C .	VAL	629	60	0.077	0.805		1.00 26.84
	3318	0	VAL	629	59	9.284	0.679		1.00 26.50
ATOM	3319	N	LEU	630		1.352	0.469		1.00 27.66
ATOM	3320	CA	LEU	630			-0.158		1.00 27.66
ATOM	3321	CB	LEU	630		3.105	0.577		
ATOM	3322	CG	LEU	630		2.856	2.086		1.00 28.00
•								-2.02/	1.00 26.06



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ATOM	3323	CD1	LEU	630	64.150	2.831	11.832	1.00	23.44
MOTA	3324	CD2	LEU	630	61.880	2.381	10.901	1.00	27.72
ATOM	3325	С	LEU	630	62.145	-1.627	12.889	1.00	32.90
ATOM	3326	0	LEU	630	62.437	-1.982	14.029	1.00	33.06
MOTA	3327	N	VAL	631	61.991	-2.478	11.873	1.00	34.83
MOTA	3328	CA	VAL	631	62.195	-3.928	12.006	1.00	33.02
ATOM	3329	CB	VAL	631	60.915	-4.700	11.584	1.00	30.92
MOTA	3330	CG1	VAL	631	61.071	-6.208	11.842	1.00	27.66
ATOM	3331	CG2	VAL	631	59.724	-4.161	12.332	1.00	24.46
ATOM	3332	С	VAL	631	63.371	-4.415	11.161	1.00	35.77
ATOM	3333	0	VAL	631	63.428	-4.171	9.954	1.00	37.57
ATOM	3334	N	THR	632	64.319	-5.098	11.797	1.00	37.96
ATOM	3335	CA	THR	632	65.511	-5.599	11.096	1.00	39.06
MOTA	3336	CB	THR	632	66.675	-5.820	12.066	1.00	35.55
MOTA	3337	OG1	THR	632	66.368	-6.903	12.955	1.00	35.76
ATOM	3338	CG2	THR	632	66.928	-4.561	12.867	1.00	35.06
ATOM	3339	С	THR	632	65.283	-6.893	10.331	1.00	40.66
ATOM	3340	0	THR	632	64.238	-7.515	10.466	1.00	41.79
MOTA	3341	N	GLU	633	66.282	-7.307	9.556	1.00	43.40
ATOM	3342	CA	GLU	633	66.219	-8.540	8.768	1.00	45.33
ATOM	3343	CB	GLU	633	67.501	-8.689	7.942	1.00	48.67
ATOM	3344	CG	GLU	633	67.496	-9.791	6.864	1.00	54.70
ATOM	3345	CD	GLU	633	66.599	-9.506	5.647	1.00	58.16
ATOM	3346	OE1	GLU	633	65.933	-8.452	5.567	1.00	60.68
ATOM	3347	OE2	GLU	633	66.566	-10.369	4.747	1.00	60.14
ATOM	3348	C	GLU	633	66.011	-9.774	9.648	1.00	46.02
MOTA	3349	0	GLU	633	65.637	-10.834	9.156	1.00	46.75
ATOM	3350	N	ASP	634	66.278	-9.648	10.944	1.00	46.45
ATOM	3351	CA	ASP	634	65.085	-10.774	11.843	1.00	46.14
ATOM	3352	CB	ASP	634	67.316	-10.995	12.724	1.00	52.89
ATOM	3353	CG	ASP	634	68.570	-11.399	11.929	1.00	59.65
MOTA	3354	OD1	ASP	634	68.593	-12.499	11.328	1.00	59.91
ATOM	3355	OD2	ASP	634	69.546	-10.608	11.918	1.00	62.29
MOTA	3356	С	ASP	634	64.850	-10.549	12.708	1.00	45.75
MOTA	3357	0	ASP	634	64.729	-11.138	13.776	1.00	46.38
ATOM	3358	N	ASN	635	63.940	-9.697	12.235	1.00	45.92
ATOM	3359	CA	ASN	635	62.690	-9.367	12.915	1.00	44.36
ATOM	3360	CB	ASN	635		-10.583	12.972	1.00	46.62
ATOM	3361	CG	ASN	635		-11.116	11.597	1.00	47.56
MOTA	3362	OD1		635		-10.453	10.800	1.00	50.54
ATOM	3363	ND2		635		-12.314	11.305	1.00	47.75
ATOM	3364	С	ASN	635	62.833	-8.763	14.308	1.00	42.78
ATOM	3365	0	ASN	635	62.028	-9.045	15.189	1.00	44.56
MOTA	3366	N	VAL	636	63.849	-7.927	14.503	1.00	41.03
ATOM	3367	CA	VAL	636	64.071	-7.291	15.797	1.00	36.87
MOTA	3368	CB	VAL	636	65.584	-7.162	16.083	1.00	
ATOM	3369	CG1		636	65.839	-6.347	17.354	1.00	34.01
ATOM	3370	CG2		636	66.184	-8.535	16.226	1.00	33.65
ATOM	3371	С	VAL	636	63.434	-5.908	15.782	1.00	
ATOM	3372	0	VAL	636	63.657	-5.131	14.854	1.00	36.58
ATOM	3373	N	MET	637	62.600	-5.625	16.773	1.00	32.04
MOTA	3374	CA	MET	637	61.940	-4.331	16.887	1.00	31.14



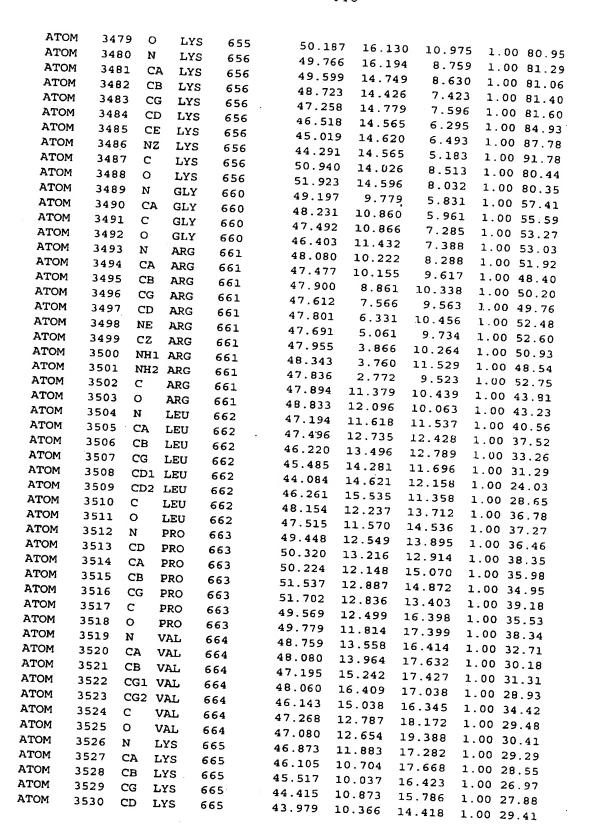
AT	_	375	CB M	ET 637	60.7	734 -4.4	127 17 2	
ATO		376	CG M	ET 637	59.7			
ATO		377	SD M	ET 637	58.8			=
ATO		378	CE M	ET 637	59.1			33.02
ATC		379	C MI	ET 637	62.9			/
ATC		880	O ME		63.5			
ATO	M 33	881	N LY	- <del>-</del> ·				
ATO	M 33	82	CA LY		63.0			1 1.00 29.03
ATO	M 33	83	CB LY	•	63.9			3 1.00 24.64
ATO.	М 33	84	CG LY		65.2			0 1.00 22.85
ATO	М 33		D LY		66.14			5 1.00 17.56
ATO			CE LY		67.30			7 1.00 19.48
ATO			Z LY		68.36			6 1.00 17.71
ATO					68.93		5 17.47	
ATOM					63.36			
ATON					62.98			
ATOM		_	'A ILI		63.27			
ATOM		_		423	62.73		6 18.536	
ATOM		-			62.69			
ATOM		-			61.91		4 20.046	
ATOM		_			62.12		0 20.963	
ATOM					60.68	0 1.39		00
MOTA		-	ILE		63.65	5 3.19		20.43
ATOM			ILE		64.884	3.16		1.00 25.36
ATOM	339	_	ALA		63.073			1.00 25.06
ATOM	340				63.857	5.037		1.00 25.70
ATOM	340				63.683	4.777		1.00 27.85
ATOM	340		ALA	•	63.380	6.449		1.00 27.66
ATOM			ALA	- <del>-</del>	62.307	6.608		1.00 29.56
ATOM	340:		ASP	641	64.174	7.456		1.00 29.82
ATOM	3404			641	63.863	8.874		1.00 28.74
ATOM	3409			641	62.662	9.310		1.00 32.13
ATOM	3406			641	63.024	9.555	14.121	1.00 35.25
ATOM	3407		1 ASP	641	64.149	9.170	13.716	1.00 38.54
ATOM	3408		2 ASP	641	62.192	10.144	13.394	1.00 39.85
ATOM	3409	_	ASP	641	63.661	9.311	17.862	1.00 41.38
ATOM	3410	_	ASP	641	63.012	10.323	18.140	1.00 30.61
ATOM	3411		PHE	642	64.265	8.567	18.776	1.00 29 45
ATOM	3412	CA	PHE	642	64.155	8.860	20.195	1.00 30.96
ATOM	3413	CB	PHE	642	64.447	7.597	21.013	1.00 31.21
	3414	CG	PHE	642	65.806	7.008	20.749	
ATOM	3415		PHE	642	66.930	7.476	21.419	1.00 24.27
ATOM	3416		PHE	642	65.962	5.978	19.838	1.00 22.36
ATOM	3417		PHE	642	68.179	6.928		1.00 24.87
ATOM	3418		PHE	642	67.205	5.420	21.190	1.00 23.19
ATOM	3419	cz	PHE	642	68.323	5.898	19.603	1.00 23.65
ATOM	3420	C	PHE	642	65.069	10.007	20.282	1.00 22.95
ATOM	3421	Ο.	PHE	642	64.920		20.623	1.00 34.88
ATOM	3422	N	GLY	643	66.000	10.549	21.729	1.00 34.84
ATOM	3423	CA	GLY	643	66.934	10.377	19.737	1.00 36.20
ATOM	3424	С ′	GLY	643	66.728	11.450		1.00 35.47
ATOM	3425	0	GLY	643	67.581	12.720	19.232	1.00 37.62
ATOM	3426	N	LEU	644		13.593	19.269	1.00 39.16
				,	65.609	12.837	18.517	1.00 39.68



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ATOM	3427	CA	LEU	644	65.328	14.029	17.712	1.00 43.09
ATOM	3428	CB	LEU	644	64.074	13.843	16.860	1.00 40.78
MOTA	3429	CG	LEU	644	64.076	12.876	15.681	1.00 36.94
MOTA	3430	CD1	LEU	644	62.790	13.076	14.901	1.00 37.34
MOTA	3431	CD2	LEU	644	65.240	13.157	14.783	1.00 37.72
ATOM	3432	C	LEU	644	65.154	15.261	18.591	1.00 47.32
ATOM	3433	0	LEU	644	64.639	15.170	19.702	1.00 50.33
ATOM	3434	N	ALA	645	65.598	16.406	18.088	1.00 51.23
ATOM	3435	CA	ALA	645	65.507	17.662	18.820	1.00 52.97
ATOM	3436	CB	ALA	645	66.367	18.703	18.151	1.00 54.12
ATOM	3437	С	ALA	645	64.060	18.137	18.910	1.00 53.00
MOTA	3438	0	ALA	645	63.591	18.528	19.977	1.00 53.59
MOTA	3439	N	ASP	652	52.356	21.675	14.855	1.00 79.51
MOTA	3440	CA	ASP	652	51.194	21.821	13.993	1.00 78.74
MOTA	3441	CB	ASP	652	51.625	22.021.	12.531	1.00 78.30
MOTA	3442	CG	ASP	652	50.459	22.358	11.608	1.00 77.64
ATOM	3443	OD1	ASP	652	49.473	22.968	12.079	1.00 77.67
ATOM	3444	OD2	ASP	652	50.526	22.029	10.410	1.00 78.25
ATOM	3445	С	ASP	652	50.339	20.569	14.125	1.00 78.92
ATOM	3446	0	ASP	652	50.645	19.529	13.539	1.00 79.36
MOTA	3447	N	TYR	653	49.262	20.682	14.892	1.00 79.17
ATOM	3448	CA	TYR	653	48.357	19.560	15.111	1.00 80.23
ATOM	3449	CB	TYR	653	47.283	19.932	16.136	1.00 81.36
ATOM	3450	CG	TYR	653	47.790	20.060	17.557	1.00 84.51
ATOM	3451	CD1	TYR	653	46.998	20.649	18.544	1.00 86.09
ATOM	3452	CE1	TYR	653	47.443	20.751	19.865	1.00 88.05
ATOM	3453	CD2	TYR	653	49.049	19.576	17.925	1.00 86.22
ATOM	3454	CE2	TYR	653	49.504	19.673	19.242	1.00 87.14
ATOM	3455	CZ	TYR	653	48.698	20.260	20.207	1.00 88.37
ATOM	3456	ОН	TYR	653	49.146	20.351	21.510	1.00 88.82
ATOM	3457	С	TYR	653	47.687	19.098	13.827	1.00 80.07
ATOM	3458	0	TYR	653	47.170	17.983	13.752	1.00 81.23
ATOM	3459	N	TYR	654	47.716	19.953	12.813	1.00 79.01
ATOM	3460	CA	TYR	654	47.082	19.640	11.544	1.00 78.81
ATOM	3461	СВ	TYR	654	46.378	20.884	11.008	1.00 78.48
ATOM	3462	CG	TYR	654	45.358	21.422	11.982	1.00 78.53
ATOM	3463	CD1	TYR	654	45.752	21.948	13.213	1.00 77.46
ATOM	3464	CE1	TYR	654	44.822	22.382	14.146	1.00 78.94
MOTA	3465	CD2	<b>T</b> YR	654	43.997	21.350	11.704	1.00 80.18
ATOM	3466	CE2	TYR	654	43.054	21.785	12.632	1.00 82.55
ATOM	3467	CZ	TYR	654	43.473	22.295	13.851	1.00 80.98
ATOM	3468	OH	TYR	654	42.548	22.703	14.785	1.00 82.29
ATOM	3469	С	TYR	654	48.010	19.042	10.499	1.00 79.04
ATOM	3470	0	TYR	654	47.575	18.720	9.393	1.00 80.09
ATOM	3471	N	LYS	655	49.277	18.859	10.848	1.00 78.74
MOTA	3472	CA	LYS	655	50.217	18.282	9.906	1.00 80.69
ATOM	3473	СВ	LYS	655	51.651	18.687	10.247	1.00 83.97
ATOM	3474	CG	LYS	655	52.674	18.124	9.281	1.00 89.76
ATOM	3475	CD	LYS	655	54.084	18.565	9.611	1.00 93.90
ATOM	3476	CE	LYS	655	55.075	17.844	8.708	1.00 97.62
ATOM	3477	NZ	LYS	655	56.489	18.177	9.038	1.00101.35
ATOM	3478	C	LYS	655	50.070	16.763	9.922	1.00 80.98
011	3410	_		0 3 3	50.070	20.703	1.246	1.00 00.90

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ATOM	3531	CE	LYS	665	42.785	11.162	13.899	1.00	26.35
ATOM	3532	NZ	LYS	665	42.363	10.809	12.508	1.00	26.16
ATOM	3533	C	LYS	665	46.890	9.730	18.556	1.00	28.81
ATOM	3534	0	LYS	665	46.315	8.802	19.113	1.00	29.38
ATOM	3535	N	TRP	666 .	48.181	9.976	18.736	1.00	28.98
ATOM	3536	CA	TRP	666	49.005	9.128	19.599	1.00	31.67
ATOM	3537	CB	TRP	666	50.323	8.755	18.913	1.00	29.46
ATOM	3538	CG	TRP	666	50.205	7.582	17.977	1.00	28.92
MOTA	3539	CD2	TRP	666	49.676	7.603	16.642	1.00	27.62
MOTA	3540	CE2	TRP	666	49.740	6.276	16.162	1.00	27.15
ATOM	3541	CE3	TRP	666	49.151	8.607	15.818	1.00	25.27
ATOM	3542	CD1	TRP	666	50.565	6.289	18.238	1.00	24.30
ATOM	3543	NEl	TRP	666	50.287	5.506	17.147	1.00	27.82
ATOM	3544	CZ2	TRP	666	49.295	5.930	14.872	1.00	26.95
ATOM	3545	CZ3	TRP	666	48.707	8.256	14.536	1.00	25.95
ATOM	3546	CH2	TRP	666	48.778	6.929	14.081	1.00	28.35
ATOM	3547	C	TRP	666	49.316	9.836	20.907	1.00	33.46
ATOM	3548	0	TRP	666	49.790	9.219	21.867	1.00	34.77
ATOM	3549	И	MET	667	49.021	11.128	20.947	1.00	35.61
MOTA	3550	CA	MET	667	49.306	11.948	22.110	1.00	37.94
MOTA	3551	CB	MET	667	49.308	13.419	21.723	1.00	40.22
MOTA	3552	CG	MET	667	50.606	13.939	21.150	1.00	40.77
MOTA	3553	SD	MET	667	50.479	15.723	20.906	1.00	44.04
MOTA	3554	CE	MET	667	50.932	15.858	19.204		39.07
MOTA	3555	C	MET	667	48.432	11.775	23.346	1.00	39.61
ATOM	3556	0	MET	667	47.211	11.672	23.255	1.00	42.46
MOTA	3557	N	ALA	668	49.072	11.820	24.505	1.00	38.46
ATOM	3558	CA	ALA	668	48.383	11.704	25.773	1.00	37.78
ATOM	3559	CB	ALA	668	49.388	11.473	26.894	1.00	38.21
ATOM	3560	С	ALA	668	47.666	13.033	25.966	1.00	37.46
ATOM	3561	0	ALA	668	48.156	14.072	25.521		35.74
MOTA	3562	N	PRO	669	46.521	13.027	26.665		37.55
ATOM	3563	CD	PRO	669	45.868	11.840	27.243		38.19
ATOM	3564	CA	PRO	669	45.723	14.229	26.923		39.30
ATOM	3565	CB	PRO	669	44.638	13.708	27.864		39.82
MOTA	3566	CG	PRO	669	44.444	12.301	27.379		39.13
ATOM	3567	C	PRO	669	46.517	15.391	27.535		40.55
ATOM	3568	0	PRO	669	46.442	16.523	27.056		39.87
MOTA	3569	N 	GLU	670	47.303	15.113	28.569		41.15
ATOM	3570	CA	GLU	670	48.096	16.169	29.200	1.00	
ATOM	3571	CB	GLU	670	48.776	15.657	30.464	1.00	
ATOM	3572	CG	GLU	670	49.928	14.705	30.205	1.00	
ATOM	3573	CD	GLU	670	49.506	13.252	30.150	1.00	
ATOM	3574	OE1		670	50.395	12.384	30.257	1.00	
ATOM	3575	OE2		670	48.297	12.974	30.013	1.00	
ATOM	3576	С	GLU	670	49.145	16.795	28.276	1.00	
ATOM	3577	0	GLU	670	49.435	17.979	28.380	1.00	
ATOM	3578	N	ALA	671	49.697	15.999	27.367	1.00	
ATOM	3579	CA	ALA	671	50.708	16.495	26.440	1.00	
ATOM	3580	CB	ALA	671	51.460	15.333	25.814	1.00	
ATOM	3581	C	ALA	671	50.063	17.364	25.361	1.00	
ATOM	3582	0	ALA	671	50.602	18.398	24.977	1.00	47.27



ATON			LEU	672	48.87	7 16.95	2 24.922	
ATOM			A LEU	672	48.13			
ATOM	-	5 C	B LEU	672	47.09			
ATOM	358	6 C	G LEU	672	46.30			
ATOM	358	7 CI	D1 LEU	672	47.23			
ATOM	358		D2 LEU		45.443			
ATOM	358	9 C	LEU		47.456			
ATOM	359	0 0	LEU	672	47.502			
MOTA	359	1 N	PHE	673	46.866			· · <b>-</b>
MOTA	359	2 CA		673			,	1.00 53.82
ATOM	3593			673	46.179	_		1.00 55.95
ATOM	3594			673	44.974	-		1.00 53.37
ATOM	3595		1 PHE	673	43.967			1.00 52.79
ATOM	3596		2 PHE		43.477	-	26.580	1.00 54.64
ATOM	3597	_	1 PHE	673	43.491		25.022	1.00 53.89
ATOM	3598			673	42.530		25.808	1.00 55.44
ATOM	3599			673	42.540		24.239	1.00 54.80
ATOM	3600			673	42.062	17.269	24.637	1.00 54.86
ATOM	3601		PHE	673	47.071	20.733	27.200	1.00 58.97
ATOM	3602		PHE	673	47.084	21.959	27.095	1.00 60.79
ATOM			ASP	674	47.832	20.086	28.077	1.00 60.63
ATOM	3603		ASP	674	48.698	20.798	29.026	1.00 61.52
ATOM	3604		ASP	674	48.638	20.137	30.410	1.00 61.39
ATOM	3605	_	ASP	674	47.247	20.143	31.010	1.00 62.87
ATOM	3606		ASP	674	46.706	19.039	31.246	1.00 62.99
	3607		2 ASP	674	46.698	21.239	31.253	1.00 63.55
ATOM	3608	C	ASP	674	50.176	20.898	28.618	1.00 61.58
ATOM	3609	0	ASP	674	51.014	21.284	29.446	1.00 60.41
ATOM	3610	N	ARG	675	50.499	20.519	27.380	1.00 61.38
ATOM	3611	CA	ARG	675	51.885	20.526	26.883	1.00 59.23
ATOM	3612	CB	ARG	675	52.336	21.944	26.515	1.00 59.05
ATOM	3613	CG	ARG	675	51.548	22.564	25.367	1.00 64.48
ATOM	3614	CD	ARG	675	52.036	23.967	25.014	1.00 68.61
ATOM	3615	NE	ARG	675	53.348	23.969	24.359	1.00 69.16
ATOM	3616	CZ	ARG	675	54.076	25.061	24.145	
ATOM	3617		ARG	675	53.622	26.250	24.531	1.00 68.19 1.00 66.97
ATOM	3618	NH2	ARG	675	55.265	24.965	23.564	
ATOM	3619	C	ARG	675	52.849	19.885	27.892	1.00 67.00
ATOM	3620	0	ARG	675	54.002	20.300	28.033	1.00 57.27
ATOM	3621	N	ILE	676	52.356	18.867	28.591	1.00 57.05
MOTA	3622	CA	ILE	676	53.136	18.140	29.589	1.00 55.44
ATOM	3623	CB	ILE	676	52.314	17.899		1.00 53.31
ATOM	3624	CG2	ILE	676	52.934	16.787	30.874	1.00 50.96
ATOM	3625	CG1	ILE	676	52.213	19.196		1.00 47.57
ATOM	3626	CD1		676	51.443			1.00 50.88
MOTA	3627	C	ILE	676	53.608	19.073		1.00 53.09
ATOM	3628	0	ILE	676				1.00 54.75
ATOM	3629	N	TYR	677	52.810			1.00 57.06
ATOM	3630		TYR	677				1.00 53.61
ATOM	3631		TYR	677				1.00 52.80
ATOM	3632		TYR	677			27.023	1.00 53.40
ATOM	3633	CD1		677			25.794	1.00 57.32
ATOM	3634	CE1					25.575	1.00 55.94
		1	_ 1 K	677	54.574	17.946		1.00 54.18

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**ATOM** 3635 CD2 TYR 677 55.140 15.251 24.829 1.00 56.63 **ATOM** 3636 CE2 TYR 677 54.459 15.654 23.680 1.00 54.84 ATOM 3637 CZTYR 677 23.490 1.00 56.38 54.183 17.004 **ATOM** 3638 OH TYR 677 53.555 17.426 22.340 1.00 57.46 **ATOM** 3639 C TYR 677 1.00 51.49 56.268 14.713 29.304 MOTA 3640 0 TYR 677 57.186 15.283 29.904 1.00 52.65 MOTA 3641 N THR 678 55.881 13.471 29.579 1.00 48.54 MOTA 3642 CA THR 678 56.571 12.648 30.568 1.00 46.14 MOTA 3643 CB THR 678 55.776 12.597 31.910 1.00 47.34 MOTA OG1 THR 3644 678 54.615 11.764 31.764 1.00 50.96 MOTA 3645 CG2 THR 678 55.346 13.996 32.345 1.00 47.47 MOTA 3646 С THR 678 56.742 11.218 3C.041 1.00 43.21 MOTA 3647 THR 678 0 56.371 10.917 28.912 1.00 41.64 MOTA 3648 N HIS 679 57.334 10.351 30.854 1.00 42.21 **ATOM** 3649 CA HIS 679 57.507 8.969 30.456 1.00 39.96 **ATOM** 3650 CB HIS 679 58.410 8.216 31,428 1.00 39.23 **ATOM** 3651 CG HIS 679 59.833 8.677 31.418 1.00 43.24 **ATOM** 3652 CD2 HIS 679 60.501 9.505 32.253 1.00 43.12 ATOM 3653 ND1 HIS 679 60.759 8.236 30.498 1.00 42.63 MOTA 3654 CE1 HIS 679 61.938 8.762 30.774 1.00 42.66 MOTA 3655 NE2 HIS 679 61.807 9.539 31.832 1.00 43.80 MOTA 3656 С HIS 679 56.145 8.301 30.429 1.00 40.78 **ATOM** 3657 0 HIS 679 55.930 7.358 29.678 1.00 42.66 ATOM 3658 N GLN 680 55.227 8.803 31.254 1.00 40.26 **ATOM** 3659 CA GLN 680 1.00 39.10 53.881 8.261 31.324 **ATOM** 3660 GLN CB 680 53.187 8.664 32.625 1.00 39.23 **ATOM** 3661 CG GLN 680 53.762 7.980 33.874 1.00 41.07 **ATOM** 3662 CD GLN 680 53.813 6.450 33.770 1.00 39.96 **ATOM** 3663 OE1 GLN 680 52.818 5.762 33.993 1.00 39.53 ATOM 3664 NE2 GLN 54.990 680 5.919 33.464 1.00 32.85 ATOM 3665 C GLN 680 53.070 8.676 30.103 1.00 39.20 ATOM 3666 0 GLN 680 52.194 7.933 1.00 39.29 29.656 ATOM 3667 N SER 681 53.368 9.843 29.531 1.00 38.01 **ATOM** 3668 CA SER 681 52.656 10.264 28.325 1.00 39.27 MOTA 3669 CB SER 681 52.979 11.712 27.968 1.00 40.93 MOTA OG 3670 SER 681 54.366 11.936 27.943 1.00 39.70 MOTA 3671 C SER 681 53.090 9.309 27.208 1.00 39.93 **ATOM** 3672 0 SER 681 52.285 8.953 26.335 1.00 40.46 MOTA 3673 N ASP 682 54.356 8.881 27.269 1.00 37.28 MOTA 3674 CA ASP 682 54.920 7.921 26.315 1.00 35.38 **ATOM** 3675 CB ASP 682 56.411 7.673 26.586 1.00 33.58 ATOM 3676 CG ASP 682 57.332 8.520 25.717 1.00 33.16 MOTA 3677 OD1 ASP 682 58.545 8.283 25.828 1.00 31.76 MOTA 3678 OD2 ASP 682 56.886 9.391 24.936 1.00 30.06 MOTA 3679 C ASP 682 54.178 6.599 26.463 1.00 34.70 **ATOM** 3680 ASP 0 682 54.012 5.868 25.488 1.00 35.67 MOTA 3681 N VAL 683 53.758 1.00 34.44 6.296 27.691 **ATOM** 3682 CA VAL 683 53.011 5.072 27.987 1.00 35.14 **ATOM** 3683 CB VAL 683 52.895 4.852 29.544 1.00 35.48 MOTA 3684 CG1 VAL 683 51.752 3.900 29.890 1.00 34.95 **ATOM** CG2 VAL 3685 683 54.202 4.282 30.080 1.00 28.77 ATOM 3686 C VAL 683 51.638 5.091 27.279 1.00 32.81

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ATOM 3687 0 VAL 683 51.173 4.050 26.801 1.00 31.24 **ATOM** 3688 N TRP 684 51.018 6.271 27.187 1.00 30.88 MOTA 3689 CA TRP 684 49.731 6.426 26.502 1.00 31.79 ATOM 3690 CB TRP 684 49.189 7.849 26.679 1.00 34.88 ATOM 3691 CG TRP 684 47.972 8.173 25.833 1.00 37.61 **ATOM** 3692 CD2 TRP 684 46.635 8.396 26.305 1.00 39.13 ATOM 3693 CE2 TRP 684 45.851 8.741 25.184 ATOM 1.00 38.42 3694 CE3 TRP 684 46.024 8.349 27.567 1.00 39.05 **ATOM** 3695 CD1 TRP 684 47.938 8.374 24.476 1.00 36.48 **ATOM** 3696 NE1 TRP 684 46.669 8.720 24.085 ATOM 1.00 38.70 3697 CZ2 TRP 684 44.483 9.036 25.290 1.00 37.82 ATOM 3698 CZ3 TRP 684 44.668 8.644 27.664 1.00 38.19 ATOM 3699 CH2 TRP 684 43.918 8.980 26.536 1.00 37.68 ATOM 3700 C TRP 684 49.947 6.131 25.020 1.00 31.09 ATOM 3701 0 TRP 684 49.214 5.332 24.430 **ATOM** 1.00 32.25 3702 N SER 685 50.977 6.750 24.444 1.00 28.90 ATOM 3703 CA SER 685 51.345 6.536 23.052 1.00 27.10 ATOM 3704 CB SER 685 52.620 7.312 22.748 ATOM 1.00 23.88 3705 OG SER 685 52.459 8.710 22.974 1.00 25.82 ATOM 3706 С SER 685 51.567 5.028 22.786 1.00 27.85 ATOM 3707 0 SER 685 51.172 4.493 21.746 1.00 28.89 MOTA 3708 N PHE 686 52.178 4.334 23.741 1.00 28.84 ATOM 3709 CA PHE 686 52.410 2.893 23.622 ATOM 1.00 27.86 3710 CB PHE 686 53.255 2.403 24.800 1.00 28.14 ATOM 3711 CG PHE 686 53.498 0.914 24.803 1.00 28.41 MOTA 3712 CD1 PHE 686 54.256 0.313 23.802 1.00 27.54 ATOM 3713 CD2 PHE 686 52.949 0.109 25.796 **ATOM** 1.00 29.15 3714 CEl PHE 686 54.465 -1.057 23.792 1.00 24.25 **ATOM** 3715 CE2 PHE 686 53.151 -1.268 25.790 1.00 27.86 MOTA 3716 CZPHE 686 53.912 -1.850 24.782 1.00 26.09 MOTA 3717 C PHE 686 51.072 2.122 23.566 1.00 30.99 ATOM 3718 0 PHE 686 50.960 1.109 22.873 1.00 29.21 ATOM 3719 N GLY 687 50.051 2.603 24.286 ATOM 1.00 30.57 3720 CA GLY 687 48.758 1.939 24.273 1.00 31.78 ATOM 3721 С GLY 687 48.202 1.923 22.862 ATOM 1.00 32.51 3722 0 GLY 687 47.687 0.908 22.373 ATOM 1.00 31.25 3723 N VAL 688 48.292 3.073 22.204 1.00 32.58 ATOM 3724 CA VAL 688 47.825 3.202 20.827 1.00 30.66 **ATOM** 3725 CB VAL 688 47.804 4.684 20.362 **ATOM** 1.00 28.55 3726 CG1 VAL 688 47.231 4.795 18.950 ATOM 1.00 27.25 3727 CG2 VAL 688 46.944 5.522 21.320 1.00 27.12 ATOM 3728 C VAL 688 48.684 2.326 19.910 1.00 29.96 ATOM 3729 0 VAL 688 48.160 1.731 18.974 1.00 30.83 ATOM 3730 N LEU 689 49.973 2.202 20.219 1.00 30.02 **ATOM** 3731 CA LEU 689 50.893 1.371 19.430 1.00 30.48 **ATOM** 3732 CB LEU 689 52.359 1.571 19.877 1.00 28.13 ATOM 3733 CG LEU 689 53.466 0.966 18.995 1.00 26.34 ATOM 3734 CD1 LEU 689 54.790 1.697 19.174 1.00 25.54 ATOM 3735 CD2 LEU 689 53.628 -0.505 19.264 1.00 24,99 MOTA 3736 C LEU 689 50.479 -0.096 19.567 1.00 30.54 MOTA 3737 0 LEU 689 50.540 -0.849 18.602 1.00 27.86 MOTA 3738 N LEU 690 50.013 -0.468 20.759 1.00 33.73

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ATOM	3739	CA	LEU	690	49.553	-1.830	21.029	1.00	32.47
ATOM	3740	CB	LEU	690	49.141	-1.982	22.496	1.00	31.82
ATOM	3741	CG	LEU	690	50.136	-2.220	23.634	1.00	29.71
ATOM	3742		LEU	690	49.396	-2.129	24.956	1.00	31.53
MOTA	3743	CD2	LEU	690	50.771	-3.605	23.483	1.00	31.69
ATOM	3744	C	LEU	690	48.335	-2.101	20.136	1.00	33.01
MOTA	3745	0	LEU	690	48.223	-3.168	19.521	1.00	32.68
ATOM	3746	N.	TRP	691	47.423	-1.131	20.089	1.00	32.37
ATOM	3747	CA	TRP	691	46.230	-1.215	19.256	1.00	32.11
ATOM	3748	CB	TRP	691	45.424	0.083	19.373	1.00	33.19
ATOM	3749	CG	TRP	691.	44.086	0.055	18.678	1.00	33.95
ATOM	3750	CD2	TRP	691	43.812	0.469	17.337	1.00	30.48
ATOM	3751	CE2	TRP	691	42.434	0.294	17.118	1.00	32.75
ATOM	3752	CE3	TRP	691	44.599	0.989	16.301	1.00	29.47
MOTA	3753	CD1	TRP	691	42.889	-0.352	19.199	1.00	34.34
ATOM	3754	NE1	TRP	691	41.894	-0.211	18.272		36.53
ATOM	3755	CZ2	TRP	691	41.831	0.601	15.900	1.00	30.85
ATOM	3756	CZ3	TRP	691	44.003	1.289	15.100	1.00	30.51
MOTA	3757	CH2	TRP	691	42.630	1.104	1.4.907		30.29
MOTA	3758	C	TRP	691	46.661	-1.421	17.805		31.49
MOTA	3759	0	TRP	691	46.062	-2.221	17.092		31.20
ATOM	3760	N	GLU	692	47.669	-0.656	17.374		32.90
ATOM	3761	CA	GLU	692	48.207	-0.734	16.019		29.78
ATOM	3762	CB	GLU	692	49.383	0.233	15.809		25.56
ATOM	3763	CG	GLU	692	49.009	1.696	15.713		25.85
ATOM	3764	CD	GLU	692	50.195	2.570	15.363		27.76
ATOM	3765	OE1	GLU	692	51.001	2.850	16.265		29.52
ATOM	3766	OE2	GLU	692	50.333	2.981	14.191		26.84
MOTA	3767	С	GLU	692	48.682	-2.136	15.696		31.08
ATOM	3768	0	GLU	692	48.545	-2.593	14.553		32.57
MOTA	3769	N	ILE	693	49.262	-2.804	16.689		31.81
ATOM	3770	CA	ILE	693	49.774	-4.163	16.506		31.87
MOTA	3771	СВ	ILE	693	50.666	-4.614	17.699		33.50
MOTA	3772	CG2	ILE	693	51.140	-6.075	17.513		33.06
MOTA	3773	CG1	ILE	693	51.879	-3.703	17.827		34.04
ATOM	3774	CD1	ILE	693	52.744	-4.008	19.025		31.52
ATOM	3775	C	ILE	693	48.643	-5.177	16.335		31.43
ATOM	3776	0	ILE	693	48.633	-5.982	15.403		29.55
MOTA	3777	N	PHE	694	47.654	-5.087	17.207		33.58
ATOM	3778	CA	PHE	694	46.550	-6.027	17.178		36.72
ATOM	3779	CB	PHE	694	45.980	-6.179	18.589		36.27
ATOM	3780	CG	PHE	694	46.988	-6.724	19.547		34.29
ATOM	3781		PHE	694	47.500	-5.949	20.581		34.95
ATOM	3782		PHE	694	47.560	-7.972	19.297		31.60
ATOM	3783	CE1		694	48.576	-6.413	21.344		35.73
ATOM	3784	CE2		694	48.633	-8.443	20.049		31.12
MOTA	3785	CZ	PHE	694	49.149	-7.661	21.066		33.97
ATOM	3786	C	PHE	694	45.516	-5.870	16.065		37.70
ATOM	3787	0	PHE	694	44.684	-6.756	15.839		37.70
ATOM	3788	N	THR	695	45.604	-4.745	15.355		
ATOM	3789	CA	THR	695	44.747	-4.485			36.11
ATOM	3790	CB	THR	695			14.205	1.00	
*** 01.1	3730	CD	Ink	093	44.107	-3.081	14.236	1.00	30.49



ATOM 3791 OG1 THR 695									
ATOM 3792 CG THR 695			3791	OG1 1	HR 695	4F 1			
ATOM 3793 C THR 695			3792						
ATOM 3794 O THR 695 ATOM 3795 N LEU 696 ATOM 3796 CA LEU 696 ATOM 3797 CB LEU 696 ATOM 3799 CG LEU 696 ATOM 3800 CD2 LEU 696 ATOM 3800 CD2 LEU 696 ATOM 3801 C LEU 696 ATOM 3801 C LEU 696 ATOM 3802 O LEU 696 ATOM 3803 C C GLY 697 ATOM 3803 CD LEU 696 ATOM 3804 CA GLY 697 ATOM 3805 C GLY 697 ATOM 3806 C GLY 697 ATOM 3807 N GLY 698 ATOM 3808 C G GLY 697 ATOM 3808 C G GLY 697 ATOM 3809 C G GLY 698 ATOM 3809 C GLY 698 ATOM 3800 C GLY 698 ATOM 3801 C GLY 698 ATOM 3801 C GLY 698 ATOM 3802 O G GLY 698 ATOM 3803 C G GLY 698 ATOM 3805 C GLY 697 ATOM 3806 C GLY 698 ATOM 3807 N GLY 698 ATOM 3808 C G GLY 698 ATOM 3808 C G GLY 697 ATOM 3809 C G GLY 698 ATOM 3809 C G GLY 698 ATOM 3800 C G GLY 698 ATOM 3801 C G GLY 698 ATOM 3801 C G GLY 698 ATOM 3802 C G GLY 698 ATOM 3803 C G GLY 698 ATOM 3803 C G GLY 698 ATOM 3804 C G G G G G G G G G G G G G G G G G G			793						512 1.00 31.07
ATOM 3795 CA LEU 696 46.859 -5.051 13.164 1.00 29.75 ATOM 3797 CB LEU 696 47.4826 -5.259 12.081 1.00 29.75 ATOM 3798 CG LEU 696 47.4826 -5.259 12.081 1.00 29.95 ATOM 3798 CG LEU 696 47.4826 -5.259 12.081 1.00 29.96 ATOM 3800 CD2 LEU 696 47.421 -8.941 10.999 1.00 30.43 ATOM 3801 C LEU 696 48.468 -8.138 12.800 1.00 32.35 ATOM 3803 N GLY 697 48.461 -4.076 11.160 1.00 28.76 ATOM 3803 N GLY 697 48.609 -1.705 10.960 1.00 32.35 ATOM 3805 C GLY 697 48.609 -1.705 10.960 1.00 32.35 ATOM 3806 CO GLY 698 46.455 -0.922 11.700 1.00 31.69 ATOM 3805 C GLY 698 45.504 1.411 11.820 1.00 31.81 ATOM 3801 N GLY 698 45.504 1.411 11.820 1.00 31.93 ATOM 3811 N SER 699 44.569 2.174 11.888 12.449 1.00 28.95 ATOM 3812 CA SER 699 44.608 3.618 11.352 1.00 31.24 ATOM 3813 CB SER 699 44.608 3.618 11.352 1.00 31.24 ATOM 3815 C SER 699 44.608 3.618 11.352 1.00 31.24 ATOM 3817 N PRO 700 44.259 4.219 10.064 1.00 31.24 ATOM 3817 N PRO 700 44.259 4.219 10.064 1.00 31.24 ATOM 3817 N PRO 700 44.259 4.219 10.064 1.00 31.24 ATOM 3817 N PRO 700 44.259 4.704 13.581 1.00 31.30 ATOM 3817 N PRO 700 44.259 4.704 13.581 1.00 31.30 ATOM 3817 N PRO 700 44.259 4.704 13.581 1.00 31.31 ATOM 3820 CB PRO 700 45.663 4.704 13.581 1.00 31.30 ATOM 3822 C PRO 700 45.663 4.704 13.593 1.00 32.27 ATOM 3822 C PRO 700 45.663 4.704 13.593 1.00 32.27 ATOM 3823 C PRO 700 45.663 4.704 13.581 1.00 31.30 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.45 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.31 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.662 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.45 1.00 30.37 ATOM 3823 C PRO 700 45.663 5.745 14.989 1.00 30.37 ATOM 3833 C PRO			794						965 1.00 29.79
ATOM 3796 CA LEU 696 ATOM 3797 CB LEU 696 ATOM 3798 CG LEU 696 ATOM 3799 CD1 LEU 696 ATOM 3800 CD2 LEU 696 ATOM 3801 C LEU 696 ATOM 3801 C LEU 696 ATOM 3803 N GLY 697 ATOM 3804 CA GLY 697 ATOM 3805 C GLY 697 ATOM 3806 C GLY 697 ATOM 3806 C GLY 697 ATOM 3807 N GLY 698 ATOM 3808 CA GLY 697 ATOM 3808 CA GLY 697 ATOM 3809 C GLY 698 ATOM 3809 C GLY 697 ATOM 3801 N GLY 698 ATOM 3808 CA GLY 697 ATOM 3808 CA GLY 697 ATOM 3808 CA GLY 697 ATOM 3808 CA GLY 698 ATOM 3809 C GLY 698 ATOM 3809 C GLY 698 ATOM 3808 CA GLY 698 ATOM 3809 C GLY 698 ATOM 3810 N SER 699 ATOM 3811 N SER 699 ATOM 3811 N SER 699 ATOM 3811 N SER 699 ATOM 3812 CA SER 699 ATOM 3813 C SER 699 ATOM 3813 C SER 699 ATOM 3816 O SER 699 ATOM 3816 C SER 699 ATOM 3817 N PRO 700 ATOM 3818 C D PRO 700 ATOM 3818 C D PRO 700 ATOM 3822 C PRO 700 ATOM 3823 C PRO 700 ATOM 3823 C PRO 700 ATOM 3824 N TYR 701 ATOM 3825 CA TYR 701 ATOM 3826 C TYR 701 ATOM 3827 CG TYR 701 ATOM 3833 C TYR 701 ATOM 3833 C TYR 701 ATOM 3834 C TYR 701 ATOM 3836 C C TYR 701 ATOM 3836 C C TYR 701 ATOM 3837 CD PRO 702 ATOM 3838 C C PRO 702 ATOM 3836 C C PRO 702 ATOM 3836 C C PRO 702 ATOM 3837 C C PRO 702 ATOM 3838		_							362 1.00 31.31
ATOM 3797 CB LEU 696 ATOM 3798 CG LEU 696 ATOM 3799 CD1 LEU 696 ATOM 3800 CD2 LEU 696 ATOM 3800 CD2 LEU 696 ATOM 3800 CD2 LEU 696 ATOM 3801 C LEU 696 ATOM 3802 C LEU 696 ATOM 3802 C LEU 696 ATOM 3803 N GLY 697 ATOM 3805 C GLV 697 ATOM 3805 C GLV 697 ATOM 3805 C GLV 697 ATOM 3806 C GLY 697 ATOM 3806 C GLY 697 ATOM 3806 C GLY 697 ATOM 3807 N GLY 697 ATOM 3808 C G GLY 697 ATOM 3808 C G GLY 697 ATOM 3809 C GLY 698 ATOM 3801 N		_	796	CA L					.64 1.00 29.75
ATOM 3799 CG LEU 696 ATOM 3800 CD2 LEU 696 ATOM 3801 C LEU 696 ATOM 3801 C LEU 696 ATOM 3802 O LEU 696 ATOM 3803 N GLY 697 ATOM 3803 N GLY 697 ATOM 3803 N GLY 697 ATOM 3806 C GLY 697 ATOM 3806 C GLY 697 ATOM 3807 N GLY 697 ATOM 3808 CA GLY 698 ATOM 3810 N GLY 698 ATOM 3810 N GLY 698 ATOM 3811 N SER 699 ATOM 3811 N SER 699 ATOM 3812 CA SER 699 ATOM 3813 CB SER 699 ATOM 3813 CB SER 699 ATOM 3814 CG SER 699 ATOM 3815 C SER 699 ATOM 3816 C SER 699 ATOM 3817 N PRO 700 ATOM 3818 CD PRO 700 ATOM 3822 C PRO 700 ATOM 3823 C PRO 700 ATOM 3823 C PRO 700 ATOM 3824 C PRO 700 ATOM 3823 C PRO 700 ATOM 3825 CA TYR 701 ATOM 3823 C PRO 700 ATOM 3823 C PRO 700 ATOM 3833 C C TYR 701 ATOM 3824 C PRO 700 ATOM 3825 CA TYR 701 ATOM 3826 C C TYR 701 ATOM 3827 CG TYR 701 ATOM 3833 C C TYR 701 ATOM 3834 C C PRO 702 ATOM 3835 C C PRO 702 ATOM 3836 C C PRO 702 ATOM 3836 C C PRO 702 ATOM 3836 C C PRO 702 ATOM 3837 CD PRO 702 ATOM 3838 C C PRO 703 ATOM 3838 C C PRO 704 ATOM 3838 C C PRO 705 ATOM 3838 C C PRO 706 ATOM 3838 C C PRO 707 ATOM 3838 C C PRO 707 ATOM 3838 C C PRO 708 ATOM 3838 C C PRO 709 A			797	CB L					1.00 28.46
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ATOM 3828 CD1 TYR 701 41.452 8.518 17.675 1.00 43.08 ATOM 3830 CD2 TYR 701 39.256 7.688 17.229 1.00 40.66 ATOM 3831 CE2 TYR 701 39.060 7.469 18.584 1.00 43.51 ATOM 3833 OH TYR 701 40.056 7.782 19.485 1.00 45.75 ATOM 3834 C TYR 701 39.847 7.592 20.837 1.00 50.92 ATOM 3835 O TYR 701 40.273 7.722 12.909 1.00 29.04 ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3838 CA PRO 702 39.761 5.346 12.186 1.00 28.69 ATOM 3839 CB PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.20		3827	CG	TYR					1.00 35.19
ATOM 3829 CE1 TYR 701 41.258 8.305 19.041 1.00 46.20 39.256 7.688 17.229 1.00 40.66 39.060 7.469 18.584 1.00 43.51 ATOM 3833 OH TYR 701 40.056 7.782 19.485 1.00 45.75 ATOM 3835 O TYR 701 40.273 7.722 12.909 1.00 29.04 ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3838 CA PRO 702 39.761 5.346 12.186 1.00 28.69 ATOM 3839 CB PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3840 CG PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.20				1 TYR					1.00 39.32
ATOM 3830 CD2 TYR 701 39.256 7.688 17.229 1.00 40.66 ATOM 3831 CE2 TYR 701 39.060 7.469 18.584 1.00 43.51 ATOM 3833 OH TYR 701 40.056 7.782 19.485 1.00 45.75 ATOM 3834 C TYR 701 40.273 7.722 12.909 1.00 50.92 ATOM 3835 O TYR 701 40.393 8.904 12.611 1.00 28.53 ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.69 ATOM 3838 CA PRO 702 39.761 5.346 12.186 1.00 26.94 ATOM 3839 CB PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 38.790 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.20		3829	CE	1 TYR					1.00 43.0B
ATOM 3831 CE2 TYR 701 39.060 7.469 18.584 1.00 40.66 ATOM 3832 CZ TYR 701 40.056 7.782 19.485 1.00 45.75 ATOM 3833 OH TYR 701 39.847 7.592 20.837 1.00 50.92 ATOM 3835 O TYR 701 40.273 7.722 12.909 1.00 29.04 ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3837 CD PRO 702 39.761 5.346 12.186 1.00 28.69 ATOM 3839 CB PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.04 ATOM 3842 O PRO 702 37.611 7.0264 1.00 29.20			CD:	2 TYR				19.041	1.00 46.20
ATOM 3832 CZ TYR 701 40.056 7.782 19.485 1.00 43.51 ATOM 3833 OH TYR 701 39.847 7.592 20.837 1.00 50.92 ATOM 3835 O TYR 701 40.273 7.722 12.909 1.00 29.04 ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3837 CD PRO 702 39.761 5.346 12.186 1.00 26.94 ATOM 3839 CB PRO 702 39.709 5.800 9.882 1.00 27.55 ATOM 3840 CG PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.20			CE:	2 TYR					1.00 40.66
ATOM 3834 C TYR 701 39.847 7.592 20.837 1.00 50.92 ATOM 3835 O TYR 701 40.273 7.722 12.909 1.00 29.04 ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3837 CD PRO 702 39.761 5.346 12.186 1.00 28.69 ATOM 3838 CA PRO 702 39.920 7.145 10.569 1.00 27.55 ATOM 3840 CG PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.04 ATOM 3842 O PRO 702				TYR		40 056			1.00 43.51
ATOM 3835 O TYR 701 40.273 7.722 12.909 1.00 29.04 ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3837 CD PRO 702 39.761 5.346 12.186 1.00 28.69 ATOM 3838 CA PRO 702 39.920 7.145 10.569 1.00 27.55 ATOM 3840 CG PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3842 O PRO 702 37.631 7.722 12.909 1.00 50.92				TYR	701				1.00 45.75
ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3837 CD PRO 702 39.761 5.346 12.186 1.00 28.69 ATOM 3838 CA PRO 702 39.920 7.145 10.569 1.00 27.55 ATOM 3840 CG PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3842 O PRO 702 37.631 7.0264 1.00 29.20			C	TYR	701				1.00 50.92
ATOM 3836 N PRO 702 40.015 6.777 11.986 1.00 28.53 ATOM 3837 CD PRO 702 39.761 5.346 12.186 1.00 26.94 ATOM 3839 CB PRO 702 39.920 7.145 10.569 1.00 27.55 ATOM 3840 CG PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3842 O PRO 702 37.631 7.0264 1.00 29.20			0	TYR					1.00 29.04
ATOM 3837 CD PRO 702 39.761 5.346 12.186 1.00 28.69 ATOM 3838 CA PRO 702 39.920 7.145 10.569 1.00 27.55 ATOM 3840 CG PRO 702 39.709 5.800 9.882 1.00 27.91 ATOM 3841 C PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3842 O PRO 702 37.631 7.0264 1.00 29.20			N	PRO					1.00 28.53
ATOM 3838 CA PRO 702 39.920 7.145 10.569 1.00 26.94 ATOM 3839 CB PRO 702 39.709 5.800 9.882 1.00 27.55 ATOM 3840 CG PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3842 O PRO 702 38.790 8.117 10.264 1.00 29.20			CD	PRO					1.00 28.69
ATOM 3839 CB PRO 702 39.709 5.800 9.882 1.00 27.55 ATOM 3840 CG PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3842 O PRO 702 38.790 8.117 10.264 1.00 29.20			CA	PRO					1.00 26.94
ATOM 3840 CG PRO 702 39.054 4.971 10.917 1.00 29.04 ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.20			CB						1.00 27.55
ATOM 3841 C PRO 702 38.790 8.117 10.264 1.00 29.04 ATOM 3842 O PRO 702 37.631 7.0029.20			CG						1.00 27.91
ATOM 3842 O PRO 702 37 631 8.117 10.264 1.00 29.20			С	PRO					1.00 29.04
7.880 10.617 1.00 32.39	ATOM	3842	0						1.00 29.20
						J / . UJI	7.880	10.617	1.00 32.39

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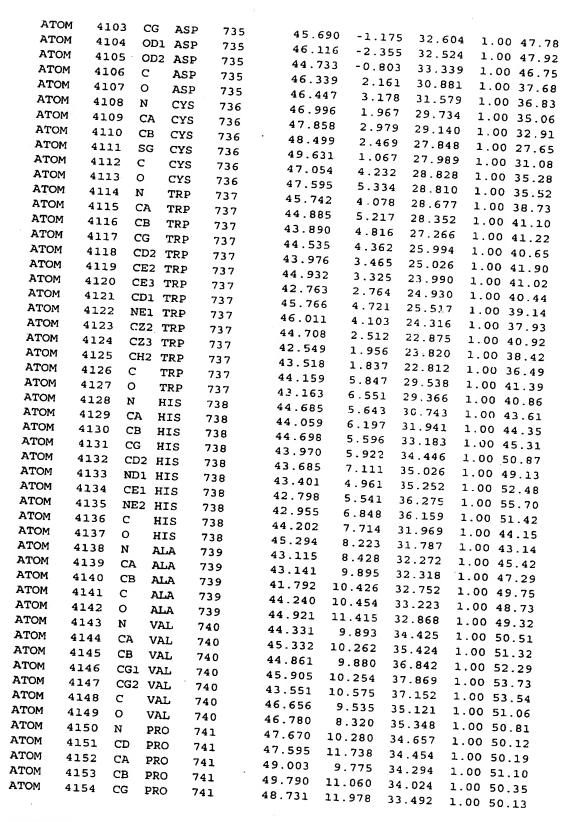
ATOM 3843 GLY 703 N 39.148 9.213 9.591 1.00 28.34 ATOM 3844 CA GLY 703 38.191 10.236 9.226 1.00 25.97 ATOM 3845 C GLY 703 37.960 11.289 10.297 1.00 28.00 **ATOM** 3846 GLY 0 703 37.175 12.213 10.079 1.00 26.40 **ATOM** 3847 N VAL 704 38.621 11.139 11.448 1.00 29.54 **ATOM** 3848 CA VAL 704 38.480 12.061 12.576 1.00 30.61 **ATOM** 3849 CB VAL 704 38.606 11.324 13.944 1.00 32.54 ATOM 3850 CG1 VAL 704 38.577 12.324 15.111 1.00 31.95 MOTA 3851 CG2 VAL 704 10.311 37.482 14.103 1.00 34.62 MOTA 3852 C VAL 704 39.490 13.210 12.557 1.00 31.37 MOTA 3853 0 VAL 704 40.683 13.001 12.757 1.00 31.73 MOTA 3854 N PRO 705 39.030 14.430 12.281 1.00 32.70 MOTA 3855 PRO CD 705 37.669 14.770 11.819 1.00 33.75 ATOM 3856 CA PRO 705 39.910 15.599 12.243 1.00 31.90 **ATOM** 3857 CB PRO 705 39.065 16.641 11.518 1.00 32.66 ATOM 3858 CG PRO 705 37.674 16.273 11.906 1.00 35.32 ATOM 3859 C PRO 705 40.331 16.053 13.635 1.00 31.85 **MOTA** 3860 0 PRO 705 39.709 15.686 14.634 1.00 31.50 **ATOM** 3861 N VAL 706 41.372 16.879 13.676 1.00 32.32 **ATOM** 3862 ÇA VAL 706 41.945 17.389 14.925 1.00 36.88 **ATOM** 3863 CB VAL 706 42.991 18.505 14.664 1.00 39.77 MOTA 3864 CG1 VAL 706 43.657 18.907 15.974 1.00 39.17 MOTA 3865 CG2 VAL 706 44.035 18.057 13.618 1.00 38.70 MOTA 3866 C VAL 706 40.938 17.923 15.953 1.00 37.80 MOTA 3867 0 VAL 706 40.994 17.581 17.140 1.00 37.45 MOTA 3868 N GLU 707 39.991 18.724 15.483 1.00 38.19 MOTA 3869 CA GLU 707 39.009 19.308 16.370 1.00 37.31 ATOM 3870 CB 38.208 GLU 707 20.361 15.619 1.00 37.46 **ATOM** 3871 C GLU 707 38.084 18.264 16.994 1.00 39.56 ATOM 3872 37.739 0 GLU 707 18.344 18.177 1.00 41.39 ATOM 3873 N GLU 708 37.724 17.260 16.206 1.00 39.99 **ATOM** 3874 CA GLU 708 36.840 16.212 16.684 1.00 40.08 **ATOM** 3875 CB GLU 708 36.334 15.377 15.515 1.00 43.96 MOTA 3876 CG GLU 708 35.505 16.163 14.496 1.00 46.61 **ATOM** 3877 CD GLU 708 34.288 16.851 15.099 1.00 52.77 **ATOM** 3878 OE1 GLU 708 33.659 16.305 16.040 1.00 52.52 ATOM OE2 GLU 3879 708 33.954 17.955 14.604 1.00 57.04 **ATOM** 3880 С GLU 708 37.551 15.337 17.704 1.00 39.89 ATOM 3881 0 GLU 708 36.944 14.900 18.684 1.00 39.47 **ATOM** 3882 N LEU 709 38.838 15.086 17.471 1.00 38.99 ATOM 3883 CA LEU 709 39.638 14.277 18.393 1.00 37.51 **ATOM** 3884 CB LEU 41.079 709 14.120 17.892 1.00 34.15 ATOM 3885 LEU CG 709 42.061 13.338 18.787 1.00 30.94 MOTA 3886 CD1 LEU 709 41.861 11.834 18.689 1.00 28.48 MOTA 3887 CD2 LEU 709 43.459 13.712 18.395 1.00 29.02 **ATOM** 3888 C LEU 709 39.644 14.961 19.751 1.00 38.18 ATOM 3889 0 LEU 709 39.460 14.313 20.787 1.00 38.08 **ATOM** 3890 N PHE 710 39.833 16.276 1.00 39.68 19.749 **ATOM** 3891 CA PHE 710 39.845 17.021 21.001 1.00 43.27 **ATOM** 3892 CB PHE 710 40.024 18.524 20.747 1.00 43.66 **ATOM** 3893 PHE CG 710 41.376 18.888 20.225 1.00 46.36 ATOM 3894 CD1 PHE 710 42.459 18.024 20.403 1.00 48.33

ATO		95	CD2 PH	E 710	41.5	79 20 00	4	
ATO		96 (	CE1 PH		43.72			
MOTA			CE2 PH		42.83			
ATON	4 38		ZZ PH		43.91			
ATOM	1 389	99 (	PH		38.55			
ATOM	1 390	00 0			38.58	_		
ATOM		)1 N		. – •		_		1.00 44.99
ATOM		2 (	A LYS		37.44			1.00 45.27
ATOM		3 C	B LYS		36.14			1.00 44.00
ATOM	390	4 C	G LYS		35.03			1.00 46.68
ATOM	390	5 C	D LYS		33.64			1.00 52.36
ATOM	390	6 C			32.55			1.00 54.43
ATOM	390				31.19			1.00 55.93
ATOM	390				30.10			1.00 63.51
ATOM	390			-	36.052	_		1.00 42.15
ATOM	391				35.635			1.00 40.85
ATOM	391:				36.467			1.00 40.98
ATOM	3912				36.432			1.00 42.26
ATOM	3913				37.012			1.00 39.67
ATOM	3914	-	1 LEU	712 712	36.159			1.00 39.06
ATOM	3915		2 LEU	712	36.899		18.504	1.00 36.97
ATOM	3916		LEU		34.842		19.857	1.00 36.48
ATOM	3917	-	LEU	712	37.232		22.974	1.00 43.61
ATOM	3918		LEU	712	36.796	11.785	23.875	1.00 44.10
ATOM	3919			713	38.407	13.141	23.038	1.00 43.57
ATOM	3920			713	39.271	13.034	24.207	1.00 43.67
ATOM	3921			713	40.619	13.726	23.958	1.00 42.24
ATOM	3922		1 LEU	713	41.569	13.004	22.989	1.00 38.81
ATOM	3923		2 LEU	713	42.856	13.796	22.817	1.00 30.86
ATOM	3924	C C	LEU	713	41.873	11.591	23.519	1.00 34.27
ATOM	3925	o	LEU	713	38.589	13.594	25.450	1.00 44.78
ATOM	3926	N	LYS	713	38.548	12.919	26.472	1.00 46.04
ATOM	3927	CA	LYS	714	38.002	14.785	25.344	1.00 44.72
ATOM	3928	CB		714	37.304	15.394		1.00 44.34
ATOM	3929	CG	LYS	714	36.818	16.799		1.00 43.76
ATOM	3930	CD	LYS	714	37.955	17.761		1.00 46.37
ATOM	3931	CE	LYS	714	37.497	19.174		1.00 52.22
ATOM	3932	NZ	LYS	714	38.701	20.044		1.00 57.37
ATOM	3933	C	LYS	714	39.792	20.059		1.00 58.02
ATOM	3934	0	LYS	714	36.142	14.534		1.00 44.17
ATOM	3935	N	LYS	714	35.861	14.499		1.00 45.14
ATOM	3936	CA	GLU	715	35.498	13.809		.00 43.86
ATOM	3937		GLU	715	34.392	12.935		.00 42.94
ATOM	3938	CB	GLU	715	33.518	12.652		.00 46.57
ATOM	3939	CG	GLU	715	32.930			.00 51.37
ATOM	3940	CD	GLU	715	32.032			.00 54.24
ATOM	3941		GLU	715	32.215			.00 54.19
ATOM	3942		GLU	715	31.139			.00 55.01
ATOM		C	GLU	715	34.878			.00 41.36
ATOM	3943	0	GLU	715	34.076			.00 38.24
ATOM	3944	N	GLY	716				.00 41.41
	3945	CA	GLY	716				
ATOM	3946	C	GLY	716	36.602			.00 41.78
								.00 42.65

MOTA	3947	0	GLY	716	36.661	7.874	27.225	1.00 41.41
ATOM	3948	N	HIS	717	36.439	9.321	25.513	1.00 44.56
ATOM	3949	CA	HIS	717	36.286	8.291	24.502	1.00 45.91
ATOM	3950	CB	HIS	717	35.935	8.926	23.153	1.00 46.65
ATOM	3951	CG	HIS	717	35.860	7.946	22.024	1.00 50.03
ATOM	3952	CD2	HIS	717	34.842	7.171	21.581	1.00 49.92
MOTA	3953		HIS	717	36.946	7.634	21.235	1.00 51.38
MOTA	3954	CEl	HIS	717	36.604	6.708	20.360	1.00 50.10
MOTA	3955	NE2	HIS	717	35.335	6.408	20.550	1.00 49.34
ATOM	3956	С	HIS	717	<b>37.53</b> 5	7.434	24.354	1.00 47.68
ATOM	3957	0	HIS	717	38.649	7.949	24.287	1.00 49.77
MOTA	3958	N	ARG	718	37.328	6.118	24.283	1.00 48.18
ATOM	3959	CA	ARG	718	38.403	5.148	24.116	1.00 46.95
ATOM	3960	CB	ARG	718	38.571	4.307	25.385	1.00 45.75
ATOM	3961	CG	ARG	718	38.945	5.125	26.618	1.00 47.15
ATOM	3962	CD	ARG	718	40.273	5.852	26.420	1.00 46.61
ATOM	3963	NE	ARG	718	40.722	6.579	27.608	1.00 45.57
ATOM	3964	CZ	ARG	718	40.601	7.896	27.779	1.00 45.48
MOTA	3965		ARG	718	40.033	8.644	26.845	1.00 44.14
ATOM	3966		ARG	718	41.122	8.480	28.854	1.00 43.32
ATOM	3967	C	ARG	718	38.109	4.250	22.912	1.00 47.56
ATOM	3968	Ò	ARG	718	36.946	3.991	22.589	1.00 48.37
ATOM	3969	N	MET	719	39.149	3.873	22.181	1.00 47.33
MOTA	3970	CA	MET	719	38.984	3.021	21.013	1.00 47.90
ATOM	3971	CB	MET	719	40.282	2.939	20.198	1.00 47.21
ATOM	3972	CG	MET	719	40.652	4.245	19.509	1.00 45.79
ATOM	3973	SD	MET	719	42.095	4.104	18.440	1.00 42.81
ATOM	3974	CE	MET	719	43.377	3.970	19.604	1.00 43.02
ATOM	3975	C	MET	719	38.519	1.629	21.392	1.00 49.99
ATOM	3976	0	MET	719	38.889	1.102	22.450	1.00 47.98
ATOM	3977	N	ASP	720	37.690	1.050	20.523	1.00 53.40
ATOM ATOM	3978	CA	ASP	720	37.135	-0.288	20.722	1.00 53.19
ATOM	3979	CB CG	ASP	720	36.089	-0.638	19.647	1.00 56.95
ATOM	3980 3981	OD1	ASP	720 ·	34.916	0.333	19.605	1.00 61.65
ATOM	3982	OD1		720 720	34.908	1.331	20.356	1.00 68.60
ATOM	3983	C	ASP	720 720	33.996	0.095	18.792	1.00 61.19
MOTA	3984	0	ASP	720	38.208 39.263	-1.372	20.713	1.00 51.12
MOTA	3985	N	LYS	720		-1.229	20.081	1.00 50.71
ATOM	3986	CA	LYS	721	37.926 38.833	-2.453 -3.576	21.432	1.00 48.85
ATOM	3987	СВ	LYS	721	38.335	-4.560	21.509 22.562	1.00 47.92 1.00 47.79
ATOM	3988	CG	LYS	721	39.024	-5.901		1.00 47.79
ATOM	3989	CD	LYS	721	38.493	-6.810	22.521 23.597	
MOTA	3990	CE	LYS	721	38.484	-8.255	23.397	1.00 53.21 1.00 54.60
ATOM	3991	NZ	LYS	721	38.158	-9.176	24.268	1.00 54.60
ATOM	3992	C	LYS	721	38.861	-4.261		1.00 61.37
ATOM	3993	0	LYS	721	37.822		20.155	
ATOM	3994	N	PRO	721	40.053	-4.688 -4.366	19.653	1.00 52.79
ATOM	3995	CD	PRO	722	41.356	-3.839	19.541	1.00 48.92
ATOM	3996	CA	PRO	722	40.167	-5.011	19.972	1.00 51.11
ATOM	3997	CB	PRO	722	41.663	-4.904	18.233	1.00 46.01
ATOM	3998	CG	PRO	722	42.090	-3.690	17.918 18.646	1.00 45.64 1.00 47.86
	5550		- 10	,	42.090	3.050	10.040	1.00 4/.86

ATO		99	C PF	20 722	39.745 -6.466 18 303 1 00 42 58
ATO	-	00	O PF		39 710 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ATO		01	N SE		39.360 -7.069 19.381 1.00 41.72
ATO		02	CA SE		7.001 17.150 1.00 43.14
ATOM		03 (	CB SE		30 360
ATOM	M 400	04 (	OG SE		29 112
MOTA	400	05 (	SE SE		39.112 -8.421 14.639 1.00 39.44
ATOM	400	06 (	SE.		40.339 -9.110 17.049 1.00 41.68
ATOM	1 400	) 7 N	I AS		41.299 -8.605 16.493 1.00 40.84
ATOM	1 400	8 0	A ASI		40.405 -10.275 17.683 1.00 45.99
ATOM	400	9 0	B ASI		41.651 -11.034 17.800 1.00 49.22
ATOM	401	.o c	G ASI		42.342 -11.215 16.453 1.00 52.35
ATOM	401	1 0	D1 ASN		41.768 -12.357 15.668 1.00 58.07
ATOM	401		D2 ASN		41.821 -13.506 16.103 1 00 62 42
ATOM					41.186 ~12.054 14.513 1 00 62 12
ATOM	401				42.558 -10.323 18.787 1.00 49.77
ATOM					43.698 -9.982 18.494 1 00 51 40
ATOM	401				41.995 -10.054 19.954 1.00 50 34
ATOM	401				42.698 -9.398 21.028 1.60 49.83
ATOM	4018				42.623 -7.878 20.868 1.00 47 11
ATOM	4019		CYS		43.485 -6.992 22.169 1.00 38 55
ATOM	4020		CYS	. – –	42.001 -9.861 22.299 1.00 50.11
ATOM	4021	_	THR		40.772 -9.852 22.383 1.00 50 63
ATOM	4022			726	42.788 -10.350 23.244 1 00 50 27
ATOM	4023			726	42.261 -10.843 24.497 1 00 51 05
ATOM	4024			726	43.341 -11.663 25.234 1 00 53 50
ATOM	4025			726	44.292 -10.780 25.829 1.00 57 56
ATOM	4026		THR	726 726	44.074 -12.554 24.241 1.00 52.55
ATOM	4027		THR	726	41.843 -9.665 25.354 1.00 52.18
ATOM	4028		ASN	726	42.403 -8.574 25.219 1.00 55 14
ATOM	4029			727	40.868 -9.860 26.237 1.00 52.55
ATOM	4030	CB	ASN	727 727	40.401 -8.781 27.114 1.00 53 17
ATOM	4031	CG	ASN		39.246 -9.265 27.992 1.00 60.65
ATOM	4032		l ASN	727	39.584 -10.545 28.751 1.00 68.99
ATOM	4033	ND		727	40.704 -10.718 29.243 1.00 73 66
ATOM	4034	C	ASN	727	38.629 -11.454 28.825 1.00 74.66
ATOM	4035	ō	ASN	727	41.537 -8.254 27.976 1.00 50.79
ATOM	4036	N	GLU	727 728	41.513 -7.107 28.414 1.00 48.17
ATOM	4037	CA	GLU	728	42.52/ -9.111 28.215 1.00 50.18
ATOM	4038	СВ	GLU		43.693 -8.764 29.020 1 00 49 60
ATOM	4039	CG	GLU	728	44.544 -10.011 29.289 1.00 50.61
ATOM	4040	CD	GLU	728	45.801 ~9.758 30.120 1.00 55 44
ATOM	4041		GLU	728	46.509 -11.045 30.542 1 00 56 45
ATOM	4042		GLU	728	46./37 -11.930 29.685 1 00 52 72
ATOM	4043	C	GLU	728	46.865 -11.161 31.733 1.00 57.38
ATOM	4044	0	GLU	728	44.509 -7.713 28.272 1.00 46.92
ATOM	4045	N		728	44.760 -6.614 28.785 1.00 46 08
ATOM	4046	CA	LEU	729	44.869 -8.039 27.033 1.00 42.69
ATOM	4047		LEU	729	45.641 -7.137 26.192 1.00 40 42
ATOM	4048	CB	LEU	729	45.950 -7.796 24.846 1.00 34 94
ATOM	4049	CG	LEU	729	47.004 -8.900 24.952 1.00 34 35
ATOM	4050		LEU	729	46.960 -9.780 23.749 1 00 31 02
	*030	CD2	ΓEΩ	729	48.404 -8.320 25.139 1.00 33.63
					2.00 33.63

MOTA	4051	С	LEU	729	44.909	-5.817	25.985	1.00 40.58
MOTA	4052	0	LEU	729	45.524	-4.760	25.929	1.00 40.10
MOTA	4053	N	TYR	730	43.591	-5.886	25.917	1.00 39.32
MOTA	4054	CA	TYR	730	42.807	-4.694	25.720	1.00 41.49
MOTA	4055	CB	TYR	730	41.384	-5.052	25.302	1.00 39.70
ATOM	4056	CG	TYR	730	40.507	-3.846	25.099	1.00 39.53
ATOM	4057	CD1	TYR	730	40.828	-2.879	24.142	1.00 35.10
ATOM	4058	CE1	TYR	730	40.019	-1.758	23.958	1.00 36.33
ATOM	4059	CD2	TYR	730	39.352	-3.661	25.874	1.00 38.44
ATOM	4060	CE2	TYR	730	38.537	-2.541	25.696	1.00 37.68
ATOM	4061	CZ	TYR	730	38.876	-1.601	24.730	1.00 36.85
MOTA	4062	ОН	TYR	730	38.041	-0.541	24.489	1.00 40.58
ATOM	4063	C	TYR	730	42.814	-3.849	26.993	1.00 43.50
ATOM	4064	0	TYR	730	42.880	-2.621	26.931	1.00 44.45
ATOM	4065	N	MET	731	42.753	-4.492	28.151	1.00 46.53
MOTA	4066	CA	MET	731	42.782	-3.744	29.406	1.00 48.67
MOTA	4067	СВ	MET	731	42.488	-4.668	30.590	1.00 54.90
ATOM	4068	CG	MET	731	41.072	-5.229	30.577	1.00 63.75
MOTA	4069	SD	MET	731	39.766	-3.998	30.763	1.00 69.82
MOTA	4070	CE	MET	731	39.849	-3.788	32.581	1.00 68.20
ATOM	4071	C	MET	731	44.148	-3.087	29.551	1.00 45.73
ATOM	4072	0	MET	731	44.273	-2.024	30.160	1.00 42.09
ATOM	4073	N	MET	732	45.168	-3.728	28.986	1.00 43.47
ATOM	4074	CA	MET	732	46.519	-3.189	29.024	1.00 43.85
ATOM	4075	CB	MET	732	47.515	-4.154	28.365	1.00 40.67
ATOM	4076	CG	MET	732	48.966	-3.646	28.369	1.00 39.96
ATOM	4077	SD	MET	732	50.252	-4.870	27.887	1.00 35,34
ATOM	4078	CE	MET	732	50.523	-5.667	29.390	1.00 35.15
ATOM	4079	C	MET	732	46.460	-1.860	28.275	1.00 43.91
ATOM	4080	0	MET	732	46.924	-0.835	28.782	1.00 47.29
ATOM	4081	N	MET	733	45.798	-1.860	27.120	1.00 42.51
ATOM	4082	CA	MET	733	45.639	-0.652	26.319	1.00 39.85
MOTA	4083	CB	MET	733	44.888	-0.932	25.013	1.00 38.08
ATOM	4084	CG	MET	733	45.614	-1.805	23.991	1.00 37.14
ATOM	4085	SD	MET	733	44.509	-2.170	22.578	1.00 37.32
MOTA	4086	CE	MET	733	45.198	-3.684	21.929	1.00 28.98
MOTA	4087	C	MET	733	44.838	0.363	27.123	1.00 41.12
ATOM	4088	0	MET	733	45.228	1.532	27.213	1.00 44.38
MOTA	4089	N	ARG	734	43.737	-0.084	27.731	1.00 40.28
MOTA	4090	CA	ARG	734	42.893	0.813	28.516	1.00 40.23
MOTA	4091	CB	ARG	734	41.632	0.095	29.007	1.00 39.95
MOTA	4092	CG	ARG	734	40.723	-0.384	27.894	1.00 36.41
ATOM	4093	CD	ARG	734	40.323	0.741	26.995	1.00 39.31
ATOM	4094	NE	ARG	734	39.510	1.733	27.682	1.00 48.97
ATOM	4095	CZ	ARG	734	38.182	1.681	27.774	1.00 53.99
ATOM	4096	NH1	ARG	734	37.503	0.681	27.222	1.00 56.64
ATOM	4097	NH2	ARG	734	37.526	2.633	28.416	1.00 56.79
MOTA	4098	C	ARG	734	43.694	1.387	29.675	1.00 39.38
MOTA	4099	0	ARG	734	43.538	2.564	30.010	1.00 41.82
ATOM	4100	N	ASP	735	44.583	0.572	30.244	1.00 37.67
MOTA	4101	CA	ASP	735	45.465	1.000	31.339	1.00 39.58
ATOM	4102	CB	ASP	735	46.392	-0.137	31.773	1.00 42.90



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MOTA 4155 C PRO 741 49.687 8.902 35.340 1.00 52.02 ATOM 4156 PRO 741 0 50.374 7.941 34.998 1.00 50.79 **ATOM** 4157 N SER 742 49.482 9.228 36.613 1.00 53.75 **ATOM** 4158 SER CA 742 50.079 8.474 37.708 1.00 54.58 **ATOM** 4159 CB SER 742 49.921 9.245 39.020 1.00 57.25 ATOM 4160 OG SER 742 48.572 9.629 39.237 1.00 61.69 **ATOM** 4161 С SER 742 49.479 7.077 37.851 1.00 53.33 ATOM 4162 0 SER 742 50.074 6.189 38.464 1.00 52.98 MOTA 4163 N GLN 743 48.286 6.897 37.305 1.00 52.97 ATOM 4164 CA GLN 743 47.616 5.613 37.390 1.00 52.15 MOTA 4165 CB GLN 743 46.108 5.827 37.505 1.00 56.12 ATOM 4166 CG GLN 743 45.506 5.374 38.838 1.00 60.50 ATOM 4167 CD GLN 743 46.269 5.887 40.046 1.00 64.45 MOTA 4168 OE1 GLN 743 46.910 5.114 40.752 1.00 65.64 ATOM 4169 NE2 GLN 743 46.199 7.194 40.290 1.00 67.99 **ATOM** 4170 С GLN 743 47.963 4.690 36.229 1.00 49.54 MOTA 4171 0 GLN 743 47.629 3.499 36.246 1.00 50.07 **ATOM** 4172 N ARG 744 48.605 5.241 35.202 1.00 46.93 **ATOM** 4173 CA ARG 744 49.010 4.437 34.044 1.00 44.51 ATOM 4174 CBARG 744 49.478 5.330 32.894 1.00 39.30 ATOM 4175 CG ARG 744 48.433 6.300 32.360 1.00 32.53 ATOM 4176 CD ARG 744 48.991 7.178 31.254 1.00 25.50 ATOM 4177 NE ARG 744 48.034 8.218 30.932 1.00 32.16 **ATOM** 4178 CZARG 744 48.352 9.454 30.542 1.00 34.35 MOTA 4179 NH1 ARG 744 49.622 9.814 30.40C 1.00 30.49 MOTA 4180 NH2 ARG 744 1.00 32.23 47.382 10.349 30.350 MOTA 4181 С ARG 744 50.153 3.498 34.472 1.00 44.61 ATOM 4182 ARG 744 О 50.833 3.741 35.474 1.00 47.68 ATOM 4183 N PRO 745 50.319 2.365 33.765 1.00 43.21 MOTA 4184 CDPRO 745 49.444 1.737 32.763 1.00 42.00 ATOM 4185 CA PRO 745 51.414 1.470 34.157 1.00 40.11 **ATOM** 4186 PRO CB 745 51.004 0.132 33.532 1.00 37.54 ATOM 4187 CG PRO 745 50.251 0.515 32.335 1.00 36.49 **ATOM** 4188 C PRO 745 52.744 1.956 33.612 1.00 39.15 **ATOM** 4189 0 PRO 745 52.807 2.654 32.602 1.00 40.56 MOTA 4190 N THR 746 53.812 1.626 34.316 1.00 37.77 ATOM 4191 CA THR 746 55.135 2.020 33.886 1.00 37.61 ATOM 4192 CB THR 746 56.113 2.132 35.091 1.00 39.14 ATOM 4193 OG1 THR 746 56.439 0.824 35.600 1.00 35.16 MOTA 4194 CG2 THR 746 55.489 2.990 36.195 1.00 36.82 ATOM 4195 C THR 746 55.687 1.036 32.852 1.00 36.75 4196 MOTA 0 THR 746 55.228 -0.103 32.772 1.00 32.89 MOTA 4197 N PHE 747 56.649 1.482 32.043 1.00 36.56 MOTA 4198 CA PHE 747 57.267 0.599 31.055 1.00 33.79 ATOM 4199 CB PHE 747 58.305 1.350 30.226 1.00 28.85 **ATOM** 4200 CG PHE 747 57.702 2.123 29.103 1.00 30.71 ATOM 4201 CD1 PHE 747 57.060 1.455 28.059 1.00 26.42 MOTA 4202 CD2 PHE 747 57.749 3.510 29.080 1.00 28.73 ATOM 4203 CE1 PHE 747 56.469 2.154 27.025 1.00 26.56 MOTA 4204 CE2 PHE 747 57.150 4.216 28.047 1.00 28.97 ATOM 4205 CZPHE 747 56.518 3.535 27.018 1.00 28 95 **ATOM** 4206 С PHE 747 57.901 -0.593 31.732 1.00 34.64

ATO	M 40	07	0 P					
ATO		08		HE 747	58.0		57 31.15 <i>6</i>	1.00 31.47
ATO		09		YS 748	58.3			
ATO				YS 748	58.9	20 -1.48		
ATO				YS 748	59.5	29 -0.95		
ATO			CG L		60.20	00 -2.04		00
			CD L		60.91			
ATO			CE L	(S 748	61.35			
ATO			NZ LY	'S 748	62.13			
ATON			C LY	S 748	57.81			0.55
ATOM			) LY	S 748	58.02			1.00 41.14
ATOM			1 GL	N 749	56.62			1.00 38.24
ATOM		18 (	CA GL	N 749	55.45		-	1.00 41.20
ATOM		.9 (	B GL		54.25			1.00 40.49
ATOM		0 0	G GL		54.37			1.00 45.70
ATOM		1 0	D GL				_	1.00 50.61
ATOM		2 0	E1 GL		53.20			1.00 55.26
ATOM	422		E2 GL		53.39			1.00 58.00
ATOM					51.988		-	1.00 59.25
ATOM	422				55.049			1.00 37.42
ATOM				_	54.964			1.00 36.00
ATOM	422				54.810		32.340	1.00 36.76
ATOM	4228			_	54.409		31.033	1.00 35.39
MOTA	4229			_	54.358		29.984	1.00 30.97
ATOM	4230				53.369			1.00 27.36
ATOM	423]		Ol LEU		53.745		29.217	1.00 29.15
ATOM	4232				51.941	-1.578	29.934	1.00 29.22
ATOM		_	LEU		55.369	-4.437	30.557	1.00 25.22
ATOM	4233	_	LEU		54.934		30.014	1.00 35.16
ATOM	4234		VAL		56.673	-4.212	30.721	
ATOM	4235	,		751	57. <b>6</b> 56	-5.217	30.312	1.00 38.76
ATOM	4236			751	59.129	-4.724	30.485	1.00 38.69
ATOM	4237		1 VAL	751	60.092	-5.836	30.120	1.00 33.81
	4238	CG	2 VAL	751	59.415	-3.535	29.598	1.00 32.04
ATOM	4239	C	VAL	751	57.428	-6.493	31.131	1.00 30.67
ATOM	4240	0	VAL	751	57.492	-7.599		1.00 41.68
ATOM	4241	N	GLU	752	57.109	-6.338		1.00 39.92
ATOM	4242	CA	GLU	752	56.854	-7.501		1.00 44.22
ATOM	4243	CB	GLU	752	56.779	-7.078		1.00 47.43
ATOM	4244	CG	GLU	752	58.093	-6.448	34.743	1.00 49.29
ATOM	4245	CD	GLU	752	58.215	-6.249		1.00 53.53
MOTA	4246	OE:	GLU	752	58.554		36.707	1.00 53.05
ATOM	4247		GLU	752	58.021	-5.123	37.136	1.00 53.63
ATOM	4248	C	GLU	752	55.594	-7.228	37.452	1.00 56.18
ATOM	4249	0	GLU	752		-8.256	32.809	L.00 46.90
ATOM	4250	N	ASP	753	55.646	-9.464	32.551	1.00 43.85
ATOM	4251	CA	ASP	753	54.490	-7.529	32.640	00 48.05
ATOM	4252	CB	ASP		53.232	-8.128	32.193 ]	.00 48.46
ATOM	4253	CG	ASP	753 753	52.119	-7.090	32.118 1	.00 51.25
ATOM	4254		ASP		51.579	-6.707	33.467 1	00 54.20
ATOM	4255		ASP	753	51.440	-7.589		.00 57.31
ATOM	4256			753	51.281	-5.513		.00 55.58
ATOM	4257	C	ASP	753	53.371			.00 48.59
ATOM		0	ASP	753	53.001			.00 49.69
01.1	4258	N	LEU	754	53.903			.00 47.21
								41.21

ATOM 4259 CA LEU 754 54.102 -8.489 28.523 1.00 46.37 **ATOM** 4260 CB LEU 754 54.664 -7.385 27.625 1.00 44.16 ATOM 4261 CG LEU 754 53.621 -6.366 27.152 1.00 46.35 MOTA 4262 CD1 LEU 754 54.296 -5.272 26.343 1.00 45.11 **ATOM** 4263 CD2 LEU 754 26.349 52.514 -7.070 1.00 42.89 ATOM 4264 С LEU 754 55.004 -9.703 28.481 1.00 47.08 MOTA 4265 0 LEU 754 54.818 -10.590 27.659 1.00 45.02 ATOM 4266 N ASP 755 55.969 -9.755 29.385 1.00 49.68 MOTA 4267 CA ASP 755 56.890 -10.876 29.487 1.00 51.62 MOTA 4268 CB **ASP** 755 57.883 -10.586 30.615 1.00 54.90 MOTA 4269 CG ASP 755 59.009 -11.589 30.702 1.00 59.00 ATOM 4270 OD1 ASP 755 59.694 -11.608 31.746 1.00 63.70 OD2 ASP MOTA 4271 755 59.223 -12.346 29.728 1.00 60.31 ATOM 4272 С **ASP** 755 56.059 -12.117 29.817 1.00 51.50 ATOM 4273 0 ASP 755 56.119 -13.150 29.138 1.00 47.11 **ATOM** 4274 N ARG 756 55.237 -11.958 30.844 1.00 51.81 ATOM 4275 CA ARG 756 31.328 54.362 -13.009 1.00 51.44 ATOM 4276 CB ARG 756 53.635 -12.519 32.582 1.00 54.52 **ATOM** 4277 CG ARG 756 52.459 -13.358 33.027 1.00 55.00 **ATOM** 4278 CD ARG 756 51.815 -12.727 34.255 1.00 59.54 **ATOM** 4279 NE ARG 756 51.417 -11.335 34.026 1.00 64.01 **ATOM** 4280 CZ ARG 756 50.366 -10.960 33.301 1.00 65.76 ATOM 4281 NH1 ARG 756 49.598 -11.866 32.721 1.00 63.56 ATOM 4282 NH2 ARG 756 50.061 -9.676 33.183 1.00 66.59 ATOM 4283 C ARG 756 53.361 -13.440 30.260 1.00 50.03 ATOM 4284 ARG 0 756 53.267 -14.622 29.960 1.00 49,98 ATOM 4285 N ILE 757 52.645 -12.483 29.673 1.00 46.87 ATOM 4286 CA ILE 757 51.656 -12.789 28.644 1.00 44.28 MOTA 4287 ILE CB 757 50.919 -11.532 28.125 1.00 40.46 ATOM 4288 CG2 ILE 757 49.923 -11.923 27.062 1.00 38.44 ATOM 4289 CG1 ILE 757 50.202 -10.830 29.277 1.00 39.74 ATOM 4290 CD1 ILE 757 49.481 -9.551 28.920 1.00 40.68 **ATOM** 4291 C ILE 757 52.251 -13.528 27.454 1.00 44.20 ATOM 4292 0 ILE 757 51.643 -14.469 26.959 1.00 40.28 MOTA 4293 N VAL 758 53.440 -13.111 27.014 1.00 47.56 ATOM 4294 CA VAL 758 54.102 -13.745 25.874 1.00 48.90 ATOM 4295 CB VAL 758 55.543 -13.177 1.00 47.01 25.609 ATOM 4296 CG1 VAL 758 56.198 -13.920 24.456 1.00 44.38 ATOM 4297 CG2 VAL 758 55.493 -11.714 25.262 1.00 47.85 ATOM 4298 C VAL 758 54.249 -15.232 26.149 1.00 51.79 ATOM 4299 VAL 0 758 54.043 -16.055 25.258 1.00 49.80 ATOM 4300 N ALA 759 54.622 -15.550 27.386 1.00 54.80 ATOM 4301 CA ALA 759 54.825 -16.925 1.00 57.15 27.814 ATOM 4302 CB ALA 759 55.406 ~16.948 29.212 1.00 56.77 ATOM 4303 С ALA 759 53.524 -17.717 27.777 1.00 60.83 ATOM 4304 0 ALA 759 53.487 -18.849 27.296 1.00 63.59 MOTA 4305 N LEU 760 52.452 -17.112 28.271 1.00 61.74 **ATOM** 4306 CA LEU 760 51.151 -17.760 28.295 1.00 61.29 MOTA 4307 CB LEU 760 50.280 -17.149 29.388 1.00 60.41 MOTA 4308 CG LEU 760 50.808 -17.323 30.812 1.00 58.68 **ATOM** 4309 CD1 LEU 760 49.917 -16.603 31.815 1.00 59.64 ATOM 4310 CD2 LEU 760 50.899 -18.799 31.138 1.00 57.84

ATO			LEU	760	50 4	39 -17.70	)	_
ATON			LEU	760		82 -18.12		
ATOM	<b>-</b>		THR	761	51 1	13 -17.20		
ATOM			THR	761	50.51	12 -17.10		
ATOM		5 CB	THR	761	50.79	94 -15.73		
ATOM		6 OG1	THR	761		93 -14.69		
ATOM		7 CG2	THR	761		02 -15.68		
ATOM		ВС	THR	761	51.20	20 -15.68	_	
ATOM		9 0	THR	761	52.03	0 -18.22	_	
ATOM	4320	) SG	CYS	1603	18.66	0 -18.49		
MOTA	432]	CG	MET	534	69.41			
ATOM	4322	SD	MET	534	69.16			
ATOM	4323	CE	MET	534	70.20			0.50 40.20
ATOM	4324	SG	CYS	603				0.50 41.95
ATOM	4325		TIP	1	56.21			0.50 37.35
ATOM	4326		TIP	2	71.86			1.00 24.40
ATOM	4327		TIP	3	39.67			1.00 36.87
ATOM	4328		TIP	4	83.769			1.00 26.81
MOTA	4329		TIP	5	83.844			1.00 30.07
ATOM	4330		TIP	6	75.192			1.00 26.76
ATOM	4331		TIP	7	86.579		-	1.00 36.11
ATOM	4332		TIP	8	52.204		24.392	1.00 36.83
ATOM	4333		TIP	9	55.174		22.514	1.00 21.93
ATOM	4334	_	rip	10	57.077		32.580	1.00 25.17
ATOM	4335		rip	11	52.281		13.300	1.00 20.79
ATOM	4336		rip		41.402		22.893	1.00 39.17
ATOM	4337	OH2		12 13	45.088		21.604	1.00 35.14
ATOM	4338		TIP		64.519		28.799	1.00 47.52
ATOM	4339	OH2 1		14	77.327		23.832	1.00 34.47
ATOM	4340		'IP	15 16	79.366	17.021	18.247	1.00 47.49
ATOM	4341		IP	17	83.087	11.573	15.986	1.00 22.80
ATOM	4342	-	IP	18	13.977	-9.804	0.222	1.00 24.88
ATOM	4343	OH2 T		20	38.451	0.155	5.081	1.00 41.03
ATOM	4344	OH2 T		21	27.109	6.286	4.902	1.00 27.69
ATOM	4345	ОН2 Т			34.379	-1.750	16.771	1.00 47.69
ATOM	4346		IP	22	20.394	2.449	27.821	1.00 54.32
ATOM	4347	OH2 T		23	50.587	-11.642	38.062	1.00 45.31
ATOM	4348		IP	24	17.137	-5. <b>94</b> 9		1.00 27.63
ATOM	4349	OH2 T		25 26	27.604	7.961	15.119	1.00 47.19
ATOM	4350	OH2 T		26	31.446	0.136		1.00 29.98
ATOM	4351	OH2 T		27 28	27.030	-13.047	27.803	1.00 28.86
ATOM		OH2 T			28.477	-17.191		1.00 37.44
ATOM		OH2 TI		29	88.748	14.279		1.00 32.72
ATOM		OH2 TI		30	-2.392	-3.684		1.00 41.86
ATOM		OH2 TI		31	34.968	-4.221		1.00 40.51
ATOM		OH2 TI		32	80.581	17.982	9.655	1.00 27.85
ATOM		OH2 TI		33	5.522	3.773	10.805	L.00 24.60
ATOM		OH2 TI		34	-10.747	5.416	11.174	1.00 29.27
		OH2 TI		35	29.049	-8.816		00 35.24
		OH2 TI		36	5.871	3.463	13.481 1	00 26.62
			_	37	31.834	2.899		00 49.70
		OH2 TI		38	19.799	2.012		.00 29.67
	-302 (	OH2 TI	P	39	62.060			.00 54.86
							_	- 51.00



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ATOM	4363	OH	TIP	40	21.100	-6.883	-4.054	1.00 22.33
MOTA	4364	OH2	TIP	41	-15.675	8.744	22.559	1.00 44.54
ATOM	4365	OH	? TIP	42	40.066	2.225	8.567	1.00 57.00
ATOM	4366	OH2	TIP	43	19.477	11.293	-0.049	1.00 37.77
ATOM	4367	OH2	TIP	44	67.060	9.047	17.334	1.00 25.14
ATOM	4368	OH2	TIP	45	87.829	18.937	18.529	1.00 45.92
ATOM	4369	OH2	TIP	46	74.741	16.956	3.987	1.00 40.33
ATOM	4370	OH2	TIP	47	29.411	16.888	10.525	1.00 38.41
ATOM	4371	OH2	TIP	48	66.592	7.020	15.108	1.00 36.15
ATOM	4372	OH2	TIP	49	85.071	21.432	5.755	1.00 19.89
ATOM	4373	OH2		50	-4.842	3.281	3.118	1.00 28.22
MOTA	4374	OH2	TIP	51	19.454	5.250	4.876	1.00 34.86
ATOM	4375	OH2	TIP	53	34.785	5.433	24.743	1.00 30.40
MOTA	4376	OH2		54	34.792	-17.150	13.665	1.00 35.81
MOTA	4377	OH2	TIP	55	59.956	7.380	27.941	1.00 36.76
ATOM	4378	OH2	TIP	56	-7.327	-1.518	6.428	1.00 39.13
MOTA	4379	OH2	TIP	57	55.164	12.120	25.338	1.00 38.87
ATOM	4380	OH2	TIP	58	68.637	6.832	16.698	1.00 54.96
ATOM	4381	OH2	TIP	59	73.778	20.869	19.031	1.00 35.01
ATOM	4382	OH2	TIP	60	3.582	-8.363	-8.103	1.00 16.71
MOTA	4383	OH2	TIP	61	38.051	10.933	5.487	1.00 32.85
ATOM	4384	OH2	TIP	62	29.727	-9.630	-1.370	1.00 30.92
MOTA	4385	OH2	TIP	64	49.186	1.253	12.066	1.00 42.67
MOTA	4386	OH2	TIP	65	41.375	3.989	28.951	1.00 37.95
MOTA	4387	OH2	TIP	66	10.798	-13.119	1.125	1.00 38.26
MOTA	4388	OH2	TIP	67	-1.079	-4.386	21.428	1.00 27.92
ATOM	4389	OH2	TIP	68	30.327	16.346	13.295	1.00 53.21
ATOM	4390	OH2	TIP	69	8.319	4.437	3.449	1.00 23.63
MOTA	4391	OH2	TIP	70	73.152	18.809	22.631	1.00 36.45
ATOM	4392	OH2	TIP	71	7.984	-3.476	25.048	1.00 33.16
ATOM	4393	он2	TIP	72 .	66.529	-4.720	28.421	1.00 66.32
ATOM	4394	OH2	TIP	73	21.577	-20.723	4.868	1.00 48.14
ATOM	4395	OH2	TIP	74	59.417	-6.760	4.957	1.00 48.73
ATOM	4396	OH2	TIP	75	16.509	-13.306	-2.942	1.00 41.02
ATOM	4397	OH2	TIP	76	-15.064	7.473	4.275	1.00 26.77
ATOM	4398	OH2	TIP	77	33.118	2.917	13.384	1.00 41.38
ATOM	4399	OH2	TIP	78	0.112	-2.913	10.809	1.00 27.49
MOTA	4400	OH2	TIP	79	17.448	2.562	5.507	1.00 16.32
ATOM	4401	OH2	TIP	81	27.445	3.796	6.134	1.00 29.83
ATOM	4402		TIP	82	-8.708	6.231	9.598	1.00 27.66
ATOM	4403		TIP	83	1.565	-1.998	8.758	1.00 33.46
ATOM	4404		TIP	84	-4.774	-3.153	7.049	1.00 36.59
ATOM .	4405	OH2		85	17.443	3.105	1.795	1.00 20.39
MOTA	4406	OH2		86	20.120	3.387	2.918	1.00 30.35
ATOM	4407	OH2		87	0.466	-2.238	22.190	1.00 20.30
ATOM	4408	OH2		88	19.749	-6.018	-1.687	1.00 21.33
ATOM	4409	OH2		89	10.505	-15.695	6.861	1.00 38.80
ATOM	4410	OH2		90	4.223	-12.113	11.774	1.00 34.18
ATOM	4411	OH2		91	6.297	1.090	-3.192	1.00 24.40
ATOM	4412	OH2		92	-13.540	1.554	5.413	1.00 34.94
MOTA	4413	OH2		93	15.607	-7.315	0.017	1.00 26.30
ATOM	4414	OH2	TIP	94	-1.868	-5.461	3.839	1.00 37.12



AT		15 OH2 T	CIP 95	10 800
ATO			'IP 96	12.718 5.095 -4.401 1.00 40.61
ATO			'IP 97	27.233 2.056 1.00 41 42
ATO		18 OH2 T		24.3/4 -13.311 0.143 1.00 52 75
ATO	OM 44	19 ОН2 Т		34.237 1.00 42 02
ATC				3.485 1.00 61.53
ATC			IP 101	73.364 -3.999 4.718 1.00 29.02
ATO		22 OH2 T		3 173 -1.967 10.565 1.00 59.23
ATO				36.623 1.00 30.51
ATO				21 102 0.620 11.780 1.00 53.77
ATO				21.408 6.462 16.955 1.00 27.62
ATO				5.552 0.791 19.345 1.00 77.65
ATO				13.000 -8.451 22.197 1.00 49.50
ATO				25 772 8.471 17.441 1.00 31.69
ATON				24.733 -10.524 -0.894 1.00 25.26
ATON		O OH2 TI		1.00 35.87
ATOM		1 OH2 TI		50.50: 12.848 3.561 1.00 35.44
ATOM	2	OH2 TI		33.384 13.491 33.225 1.00 40.47
ATOM	_	OH2 TI		8 022 2 2 2 1.00 47.07
ATOM		OH2 TI	2 114	75 205 -1710 0.940 1.00 40.79
ATOM		OH2 TI	115	40 000 1- 100 55.51
ATOM			116	2 722 1.00 38.97
ATOM			117	2.333 -11.271 9.174 1.00 38.97 83.062 26.404 12.825 1.00 29.12
ATOM			118	8 916 5 113
ATOM	4439		119	-8.504 4.55
ATOM	4440			7 505 13 755
ATOM	4441	OH2 TIP		51 500 6 55
ATOM	4442	OH2 TIP	122	20 720 2 21 20 25.18
ATOM	4443	OH2 TIP	123	73 111 2 222
ATOM	4444	OH2 TIP	124	5 312 11 500
ATOM ATOM	4445	OH2 TIP	125	34 207 2 42-
	4446	OH2 TIP	126	0 535 75 75 75 75 75 75 75 75 75 75 75 75 75
ATOM ATOM	4447	OH2 TIP	127	8 227
ATOM	4448	OH2 TIP	129	17 312 7 22
ATOM	4449	OH2 TIP	130	35 924 3 665
ATOM	4450	OH2 TIP	131	44 722 10 205
ATOM	4451	OH2 TIP	132	27 941 12 15
ATOM	4452	OH2 TIP	133	45 301 11 12
ATOM	4453	OH2 TIP	134	57 705 30 35.00
ATOM	4454	OH2 TIP	135	-3 100 15 200
ATOM	4455	OH2 TIP	136	95 904 37 27 27
ATOM	4456	OH2 TIP	137	12 840 2 1.00 32.04
ATOM	4457	OH2 TIP	138	75 545 2 2 2 2 2 3 2 3 0 . 08
ATOM	4458	OH2 TIP	139	13 020 7 7 7 1.00 33.94
ATOM	4459	OH2 TIP	140	11 245 10 25 1.00 40.68
ATOM		OH2 TIP	141	59 563 70 663
ATOM ATOM		OH2 TIP	142	13 671 76 71 34
ATOM		OH2 TIP	143	-6 350
ATOM ATOM		OH2 TIP	144	25 620 37.08
ATOM ATOM		OH2 TIP	145	-16 450 30.51
ATOM		OH2 TIP	146	85 500 10 0.324 1.00 38.40
-1011	4466	OH2 TIP	147	32 120 1.00 47.80
				32.139 ~4.674 1.757 1.00 32.43

MOTA	4467	OH2 TI	P 148	44.890	7.505	11.806	1.00 32.46
MOTA	4468	OH2 TI	P 149	80.781	12.432	16.562	1.00 47.77
ATOM	4469	OH2 TI	P 150	3.017	-7.101	-1.917	1.00 40.92
MOTA	4470	OH2 TI	P 151	31.784	-6.139	20.968	1.00 38.23
MOTA	4471	OH2 TI	P 152	74.835	-2.597	12.290	1.00 48.89
MOTA	4472	OH2 TI	P 153	7.509	6.768	-1.083	1.00 46.02
ATOM	4473	OH2 TI	P 154	71.732	5.360	21.908	1.00 33.30
MOTA	4474	OH2 TI	155	68.150	-5.075	8.794	1.00 39.31
ATOM	4475	OH2 TI		0.148	-9.544	6.872	1.00 41.37
MOTA	4476	OH2 TI		67.878	18.204	10.861	1.00 51.19
ATOM	4477	OH2 TI	158	3.652	8.829	4.428	1.00 31.24
ATOM	4478	OH2 TI	2 159	52.100	11.362	18.433	1.00 40.73
MOTA	4479	OH2 TI	2 161	-10.357	6.783	4.861	1.00 35.13
MOTA	4480	OH2 TI	162	76.471	1.562	-0.853	1.00 59.17
MOTA	4481	OH2 TIE	163	10.073	-12.056	17.071	1.00 44.69
ATOM	4482	OH2 TI	164	34.163	14.271	18.254	1.00 39.59
ATOM	4483	OH2 TI		2.320	-7.990	16.820	1.00 38.19
ATOM	4484	OH2 TIE		29. <b>69</b> 6	1.908	6.098	1.00 38.02
ATOM	4485	OH2 TIE	167	32.626	-17.410	11.766	1.00 48.15
MOTA	4486	OH2 TIP	168	42.244	18.049	11.043	1.00 50.95
ATOM	4487	OH2 TIP	169	87.907	10.574	5.721	1.00 60.28
ATOM	4488	OH2 TIP		70.313	3.998	25.141	1.30 72.64
MOTA	4489	OH2 TIP	171	77.603	5.679	23.952	1.00 43.23
ATOM	4490	OH2 TIF	172	-0.942	-8.153	4.508	1.00 55.10
ATOM	4491	OH2 TIF		34.297	15.574	1.690	1.00 34.19
ATOM	4492	OH2 TIP		-9.643	7.829	7.414	1.00 50.48
ATOM	4493	OH2 TIP		11.618	5.655	7.455	1.00 43.37
MOTA	4494	OH2 TIP		-8.705	13.841	13.642	1.00 72.49
ATOM	4495	OH2 TIP		32.009	3.416	18.257	1.00 44.16
ATOM	4496	OH2 TIP		-8.651	10.180	24.352	1.00 44.85
ATOM	4497	OH2 TIP		-1.153	-6.532	15.548	1.00 32.90
ATOM	4498	OH2 TIP		80.235	0.749	15.508	1.00 34.75
ATOM	4499	OH2 TIP		67.222	20.490	-1.574	1.00 40.76
ATOM	4500	OH2 TIP		-0.471	4.367	1.248	1.00 36.58
MOTA	4501	OH2 TIP		0.149	6.517	2.578	1.00 40.12
ATOM	4502	OH2 TIP		-1.186	8.867	1.311	1.00 44.77
ATOM	4503	OH2 TIP		-5.093	9.260	2.252	1.00 52.07
ATOM	4504	OH2 TIP		-7.235	10.227	3.913	1.00 58.53
ATOM	4505 4506	OH2 TIP		2.724	7.169	0.879	1.00 47.77
ATOM ATOM		OH2 TIP		5.527	11.031	8.519	1.00 34.40
ATOM	4507 4508	OH2 TIP		63.927	12.721	22.689	1.00 40.75
ATOM		OH2 TIP		79.264	1.066	18.321	1.00 41.34
MOTA	4509 4510	OH2 TIP				7.256	1.00 79.86
ATOM	4510	OH2 TIP		13.994	-0.972	-4.310	1.00 31.15
ATOM	4511	OH2 TIP	193	59.546	3.024	33.227	1.00 40.34
	4512	OH2 TIP	194	32.179	13.637	19.964	1.00 48.25
ATOM	4513	OH2 TIP	195	72.178	16.188	22.879	1.00 42.72
ATOM	4514	OH2 TIP	196	0.898	-8.663	14.348	1.00 41.76
ATOM	4515	OH2 TIP	197	-0.490	5.455	30.574	1.00 38.30
ATOM	4516	OH2 TIP	199	-1.277	-4.244	27.691	1.00 56.27
ATOM ATOM	4517	OH2 TIP	200	81.605	15.360	17.272	1.00 42.05
ALOM	4518	OH2 TIP	201	-17.534	4.081	23.779	1.00 59.65

ATO		OH2 TI	P 202	27.748 10.634 14.595 1.00.48.07
ATO		OH2 TI	P 203	34 991 4 459 1.00 49.97
ATO		OH2 TI	P 204	-3 460 4
ATO		OH2 TI		9.045 1.00 44.70
ATO		OH2 TI	P 206	
ATO	M 4524	OH2 TI		1.00 35.12
OTA	M 4525	OH2 TI		26.871 14.098 19.820 1.00 53.04
ATOM	M 4526	OH2 TI		9.323 6.370 1.00 37.49
ATON	4527	OH2 TI		55.553 15.911 1.00 72.92
ATOM	1 4528	OH2 TIP		55.080 15.928 20.414 1.00 68.75
ATOM	1 4529	OH2 TIP		31.312 19.264 22.672 1.00 54.72
ATOM	1 4530	OH2 TIP		19.988 7.127 6.976 1.00 45.55
ATOM		OH2 TIP		28.905 2.021 -3.430 1.00 48.55
ATOM		OH2 TIP		20.446 2.593 -4.753 1 00 55 04
ATOM		OH2 TIP	_	36.539 2.911 18.446 1 00 38 50
ATOM		OH2 TIP	·	16.807 -20.725 14.119 1 00 56 02
ATOM		OH2 TIP		28.203 -14.485 6.172 1 00 62 00
ATOM	_	OH2 TIP	_	31.519 1.503 -2.010 1 00 56 10
ATOM		OH2 TIP		10.014 -16.571 15.451 1 00 46 27
ATOM			220	7.126 -11.922 5.526 1 00 56 00
ATOM		OH2 TIP	221	-12.414 14.643 10.965 1 00 67 36
ATOM		OH2 TIP	222	10,978 9.734 -1,436 1 00 38 91
ATOM		OH2 TIP	223	11.293 12.362 -1.306 1.00 52.56
ATOM		OH2 TIP	224	34.011 13.162 -1.255 1.00 52.58
ATOM		OH2 TIP	225	31.195 17.923 8.021 1.00 75.88
ATOM		OH2 TIP	226	36.957 11.949 -1.947 J.00 50.99
ATOM		OH2 TIP	227	35.179 3.114 10.888 1.00 58.55
ATOM	_	OH2 TIP	228	64.027 13.281 26.577 1.00 51.98
ATOM		H2 TIP	229	36.514 6.155 15.292 1.00 45.57
ATOM		H2 TIP	230	90.627 4.339 6.386 1.00 56.65
ATOM		H2 TIP	231	49.907 -11.937 10.792 1.00 53.49
ATOM	-	H2 TIP	232	60.296 -10.212 16.610 1.00 79.85
ATOM		H2 TIP	233	18.154 -21.314 7.018 1.00 53.60
ATOM	-	H2 TIP	234	66.186 -1.068 30.882 1.00 56.92
ATOM		H2 TIP	235	75.153 18.983 20.700 1.00 34.22
ATOM		H2 TIP	236	-3 000 10 000
ATOM		H2 TIP	237	5 934 3 50
ATOM		H2 TIP	238	35 970 6 465
ATOM		H2 TIP	239	-E 404 36 55-
ATOM		H2 TIP	240	46 333 33 603
		H2 TIP	241	6 170
ATOM		12 TIP	242	1.00 45.92
ATOM		12 TIP	243	1 (2)
ATOM		12 TIP	244	96 101 1.00 41.42
ATOM		2 TIP	245	10 501 5 5.22
ATOM		2 TIP	246	E 007 0 107 1.00 77.40
ATOM		2 TIP	247	64 553
ATOM		2 TIP	248	17 242 17 655
ATOM		2 TIP	249	12 226
ATOM	4567 OH	2 TIP	250	2 075
ATOM		2 TIP	251	72 040
MOTA		2 TIP	252	50 353
ATOM		2 TIP	254	F7 700 67.13
				57.772 9.500 11.808 1.00 40.03



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MOTA	4571	OH2	TIP	255	43.306	20.459	30.366	1.00	47.59
MOTA	4572	OH2	TIP	256	67.064	16.514	15.765	1.00	57.51
MOTA	4573	OH2	TIP	257	87.612	21.648	5.147	1.00	70.52
MOTA	4574	OH2	TIP	258	21.095	9.853	-9.308	1.00	78.97
MOTA	4575	OH2	TIP	261	71.914	28.544	7.912	1.00	83.90
MOTA	4576	OH2	TIP	262	25.727	-8.133	27.190	1.00	54.87
MOTA	4577	OH2	TIP	263	-18.738	10.877	12.767	1.00	71.80
MOTA	4578	OH2	TIP	264	30.524	11.543	16.329	1.00	46.98
MOTA	4579	OH2	TIP	265	22.211	-16.242	-2.763	1.00	55.17
MOTA	4580	OH2	TIP	266	29.755	9.037	18.396	1.00	67.93
ATOM	4581	C1	MON	1000	67.458	4.500	11.935	1.00	0.00
ATOM	4582	C2	MON	1000	67.015	3.958	10.687	1.00	0.00
ATOM	4583	NЗ	MON	1000	67.367	2.732	10.160	1.00	0.00
ATOM	4584	C4	MON	1000	66.127	4.618	9.793	1.00	0.00
ATOM	4585	C5	MON	1000	65.620	5.919	10.125	1.00	0.00
ATOM	4586	C6	MON	1000	66.041	6.508	11.380	1.00	0.00
ATOM	4587	C7	MON	1000	66.948	5.809	12.276	1.00	0.00
MOTA	4588	C8	MON	1000	65.933	3.759	8.668	1.00	0.00
ATOM	4589	C10	MON	1000	66.745	2.518	8.922	1.00	0.00
MOTA	4590	C11	MON	1000	65.043	4.051	7.483	1.00	0.00
ATOM	4591	012	MON	1000	66.862	1.516	8.241	1.00	0.00
ATOM	4592	C13	MON	1000	64.479	2.990	6.570	1.00	0.00
ATOM	4593	C14	MON	1000	63.459	3.330	5.617	1.00	0.00
ATOM	4594	C15	MON	1000	62.923	2.333	4.727	1.00	0.00
MOTA	4595	C16	MON	1000	63.379	0.956	4.754	1.00	0.00
ATOM	4596	C17	MON	1000	64.960	1.637	6.605	1.00	0.00
ATOM	4597	C18	MON	1000	64.418	0.642	5.713	1.00	0.00
ATOM	4598	N19	MON	1000	62.848	-0.025	3.880	1.00	0.00
ATOM	4599	C20	MON	1000	63.429	-1.407	3.816	1.00	0.00
ATOM	4600	C21	MON	1000	61.888	0.343	2.786	1.00	0.00
MOTA	4601	C22	MON	1000	61.085	-0.818	2.152	1.00	0.00
MOTA	4602	N23	MON	1000	61.868	-2.035	1.930	1.00	0.00
MOTA	4603	C24	MON	1000	62.562	-2.492	3.133	1.00	0.00
ATOM	4604		MOM	1000	61.481	-2.328	-0.389	1.00	0.00
ATOM	4605		MON	1000	62.001	-2.670	0.659	1.00	0.00
ATOM	4606	Cl	MON	1001	5.458	3.340	18.422	1.00	0.00
ATOM	4607	C2	MON	1001	6.049	3.475	19.718	1.00	0.00
ATOM	4608	И3	MON	1001	5.935	2.580	20.763	1.00	0.00
ATOM	4609	C4	MON	1001	6.857	4.573	20.124	1.00	0.00
ATOM	4610	C5	MON	1001	7.121	5.641	19.202	1.00	0.00
ATOM	4611	C6	MON	1001	6.543	5.548	17.877	1.00	0.00
MOTA	4612	C7	MON	1001	5.722		17.489	1.00	0.00
MOTA	4613	C8	MON	1001	7.250	4.340	21.477	1.00	0.00
ATOM	4614		MOM	1001	6.647	3.023	21.886	1.00	0.00
ATOM	4615		MON	1001	8.138	5.242	22.302	1.00	0.00
ATOM	4616	012		1001	6.735	2.426	22.943	1.00	0.00
MOTA	4617	C13		1001	8.918	4.783	23.509	1.00	0.00
ATOM	4618		MON	1001	9.913	5.641	24.091	1.00	0.00
MOTA	4619		MON	1001	10.654	5.224	25.253	1.00	0.00
ATOM	4620		MON	1001	10.435	3.935	25.881	1.00	0.00
ATOM	4621		MON	1001	8.670	3.508	24.123	1.00	0.00
ATOM	4622	C18	MON	1001	9.416	3.095	25.285	1.00	0.00

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4623 4624 4625 4626 4627 4628 4629 4630	N19 MON C20 MON C21 MON C22 MON N23 MON C24 MON O25 MON C26 MON	1001	11.168 10.831 12.107 13.125 12.570 11.902 13.118 12.610	3.525 2.255 4.463 3.821 2.742 1.711 3.569 2.731	27.023 27.749 27.725 28.698 29.518 28.725 31.669	1.00 1.00 1.00 1.00 1.00 1.00	0.00 0.00 0.00 0.00 0.00 0.00
				12.610	2.731	30.944	1.00	0.00

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#### CLAIMS

What is claimed is:

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1. A crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

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2. The crystalline form of claim 1, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

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3. The crystalline form of claim 2, wherein said receptor protein tyrosine kinase is selected from the group consisting of PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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4. The crystalline form of claim 1, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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5. The crystalline form of claim 4, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

6. The crystalline form of claim 1, comprising one or more heavy metal atoms.

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7. The crystalline form of claim 1, wherein said

protein tyrosine kinase is FGFR.

8. The crystalline form of claim 7, wherein said FGFR is FGFR1.

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- 9. The crystalline form of claim 8, defined by atomic structural coordinates set forth in Table 1.
- 10. The crystalline form of claim 7, comprising at least one compound.
  - 11. The crystalline form of claim 10, wherein said compound is a nucleotide analog.

12. The crystalline form of claim 11, wherein said nucleotide analog is AMP-PCP.

- 13. The crystalline form of claim 12, defined by atomic structural coordinates set forth in Table 2.
- 14. The crystalline form of claim 10, wherein said compound is an indolinone compound.
- 15. The crystalline form of claim 14, wherein said indolinone compound has a structure set forth in formula I or II:

$$R_{3}$$

$$R_{4}$$

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{4}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

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$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

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$$R_{3}$$

$$R_{4}$$

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

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$$R_{3}$$

$$R_{4}$$

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_{5}$$
 $A_{2}$ 
 $A_{1}$ 
 $R_{6}$ 
 $A_{3}$ 
 $A_{4}$ 
 $R_{7}$ 
 $R_{1}$ 
 $R_{1}$ 
 $R_{1}$ 
 $R_{2}$ 

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

- (a)  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are independently carbon or nitrogen;
  - (b) R<sub>1</sub> is hydrogen or alkyl;
- (c)  $R_2$  is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
  - (d) R<sub>3</sub> is hydrogen;
  - (e)  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  are optionally present and are

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either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(0)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R,  $(CH_2)_nCO_2R$ , and CONRR' or (ii) any two adjacent  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

- (f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each
  independently selected from the group consisting of
  hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl,
  alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R,
  SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R,
  and CONRR';
- 15 (g) n is 0, 1, 2, or 3;
  - (h) R is hydrogen, alkyl or aryl;
  - (i) R' is hydrogen, alkyl or aryl; and
- (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, 20 pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 25 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R,  $(CH_2)_nCO_2R$  or CONRR'. 30



16. The crystalline form of claim 15, wherein said indolinone compound is 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone.

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17. The crystalline form of claim 15, wherein said indolinone compound is 3-[4-(4-formylpiperazine-1-yl)benzylidenyl]-2-indolinone.

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18. The crystalline form of claim 16, defined by the atomic structural coordinates of Table 3.

19. The crystalline form of claim 17, defined by the atomic structural coordinates of Table 4.

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20. The crystalline form of claim 1, having monoclinic unit cells.

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21. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and  $\beta$ =107.2°.

22. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and  $\beta$ =107.7°.

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23. The crystalline form of claim 10, comprising one or more heavy metal atoms.

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24. A polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first



glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal boundary of the catalytic domain.

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25. The polypeptide of claim 24, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

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26. The polypeptide of claim 24, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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27. The polypeptide of claim 25, wherein said receptor tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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28. The polypeptide of claim 26, wherein said non-receptor kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

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- 29. The polypeptide of claim 24 having the amino acid sequence shown in SEQ ID NO:4.
- 30. A method of using the polypeptide of claim 24 to form a crystal, comprising the steps of:
- (a) mixing a volume of polypeptide solution with a reservoir solution; and

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(b) incubating the mixture obtained in step(a) over the reservoir solution in a closed container,

under conditions suitable for crystallization.

- 31. A method of obtaining an FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of:
- (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, wherein said polypeptide solution comprises 1 mg/mL to 60 mg/mL FGF-type tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and wherein said reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and
- (a) over said reservoir solution in a closed container at a temperature between 0° and 25° °C until crystals form.

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32. The method of claim 31, wherein said polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

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33. The method of claim 31, wherein said

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polypeptide solution comprises a compound.

- 34. A cDNA encoding an FGF receptor tyrosine kinase domain protein, wherein a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.
- 35. A method of determining three dimensional structures of protein tyrosine kinases with unknown structure comprising the step of applying structural atomic coordinates set forth in Table 1, Table 2, Table 3, or Table 4.
- 36. The method of claim 35, comprising the following steps:
- (a) aligning a first computer representation of an amino acid sequence of a protein tyrosine kinase of unknown structure with a second computer representation of a protein tyrosine kinase of known structure by matching homologous regions of amino acid sequences of said first computer representation and said second computer representation;
- (b) transferring computer representations of amino acid structures in said protein tyrosine kinase of known structure to computer representations of corresponding amino acid structures in said protein tyrosine kinase with unknown structure; and
- (c) determining a low energy conformation of the protein tyrosine kinase structure resulting from step (b).
  - 37. The method of claim 35, comprising the

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following steps:

- (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals; and
- (b) determining a low energy conformation of the resulting protein tyrosine kinase structure.
- 38. The method of claim 35, comprising the following steps:
- (a) determining the secondary structure of a protein tyrosine kinase structure using NMR data; and
- (b) simplifying the assignment of throughspace interactions of amino acids.
- 39. The method of any one of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a receptor protein tyrosine kinase.
- 20 protein tyrosine kinase with or without known structure is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.
- 41. The method of anyone of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a non-receptor protein tyrosine kinase.
- 42. The method of claim 41, wherein said protein tyrosine kinase with or without known structure is

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selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

- 43. A method of identifying a potential modulator of protein tyrosine kinase function by docking a computer representation of a structure of a compound with a computer representation of a structure of a cavity formed by the active-site of a protein tyrosine kinase, wherein said structure of said protein tyrosine kinase is defined by atomic structural coordinates set forth in Table 1, Table 2, Table 3, or Table 4.
- 44. The method of claim 43, comprising the following steps:
- (a) removing a computer representation of a compound complexed with a protein tyrosine kinase and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the protein tyrosine kinase;
- (b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and
- (c) identifying compounds that best fit said active-site as potential modulators of protein tyrosine kinase function.
- 45. The method of claim 43, comprising the following steps:
- (a) modifying a computer representation of compound complexed with a protein tyrosine kinase by the deletion of a chemical group or groups or by the

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addition of a chemical group or groups;

- (b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and
- (c) identifying compounds that best fit the protein tyrosine kinase active-site as potential modulators of protein tyrosine kinase function.
- 46. The method of claim 43, wherein said method comprises the following steps:
- (a) removing a computer representation of a compound complexed with a protein tyrosine kinase; and
- (b) searching a data base for data base compounds similar to said compounds using a compound searching computer program or replacing portions of said compound with similar chemical structures from a data base using a compound construction computer program.
- 47. The method of any one of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.
  - 48. The method of claim 47, wherein said receptor protein tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.
  - 49. The method of anyone of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

- 50. The method of claim 49, wherein said protein tyrosine kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.
- 5 51. a potential modulator of protein tyrosine kinase function identified by the method of any one of claims 43, 44, 45, or 46.
  - 52. The potential modulator of claim 51, wherein said modulator is selected from a computer data base.
  - 53. The potential modulator of claim 51, wherein said modulator is constructed from chemical groups selected from a computer data base.
  - 54. The potential modulator of protein tyrosine kinase function of claim 51, wherein said modulator is an indolinone compound of formula I or II:

$$R_{5}$$
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 $R_{5}$ 
 $R_{6}$ 
 $R_{6}$ 
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R

(I)

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$$R_{5}$$
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 $A_{7$ 

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

- (a)  $A_1$ ,  $A_2$ ,  $A_3$ , and  $A_4$  are independently carbon or nitrogen;
  - (b) R<sub>1</sub> is hydrogen or alkyl;
- (c)  $R_2$  is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
  - (d) R<sub>3</sub> is hydrogen;

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(e)  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  are optionally present and are either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(0)R,  $SO_2NRR'$ ,  $SO_3R$ , SR,  $NO_2$ , NRR', OH, CN, C(0)R, OC(0)R, NHC(0)R,  $(CH_2)_nCO_2R$ , and CONRR' or (ii) any two adjacent  $R_4$ ,  $R_5$ ,  $R_6$ , and  $R_7$  taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

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(f) R<sub>2</sub>', R<sub>3</sub>', R<sub>4</sub>', R<sub>5</sub>', and R<sub>6</sub>' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R,

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SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R,  $(CH_2)_nCO_2R$ , and CONRR';

- (g) n is 0, 1, 2, or 3;
- (h) R is hydrogen, alkyl or aryl;
- (i) R' is hydrogen, alkyl or aryl; and
- (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO<sub>2</sub>NRR', SO<sub>3</sub>R, SR, NO<sub>2</sub>, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R or CONRR'.
- 55. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, comprising the following steps:
  - (a) administering said potential modulator to cells;
  - (b) comparing the level of protein tyrosine kinase phosphorylation between cells not administered the potential modulator and cells administered said potential modulator; and
- (c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on

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the difference in the level of protein tyrosine kinase phosphorylation.

- 56. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, wherein said method comprises the following steps:
- (a) administering a preparation of saidpotential modulator to cells;
- (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and
- (c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on the difference in the rate of cell growth.
- 57. A method of treating a disease associated with a protein tyrosine kinase with inappropriate activity in a cellular organism, wherein said method comprises the steps of:
- (a) administering a modulator of protein tyrosine kinase function to the organism, wherein said modulator is in an acceptable pharmaceutical preparation; and
- (b) activating or inhibiting the protein tyrosine kinase function to treat the disease.
- 58. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

- 59. The method of claim 58, wherein said receptor protein tyrosine kinase is selected from the group containing FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.
- 60. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.
- 61. The method of claim 60, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

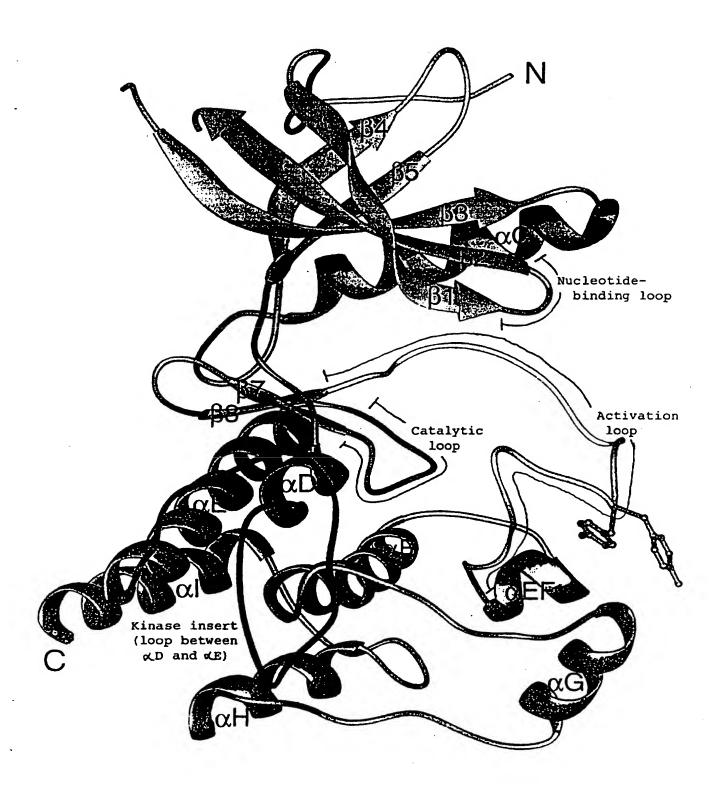
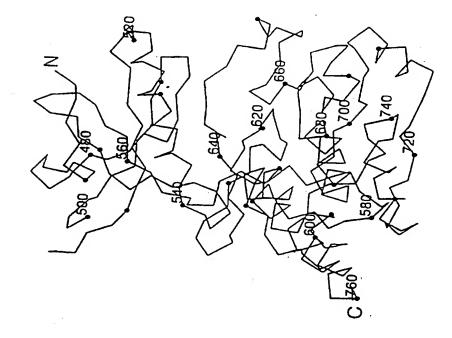


FIGURE 1





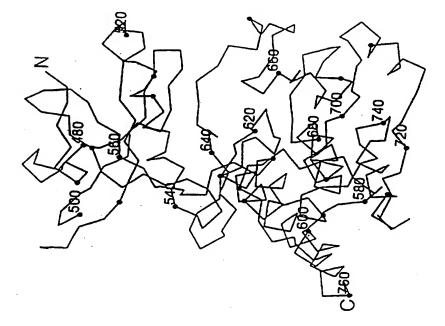
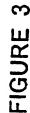
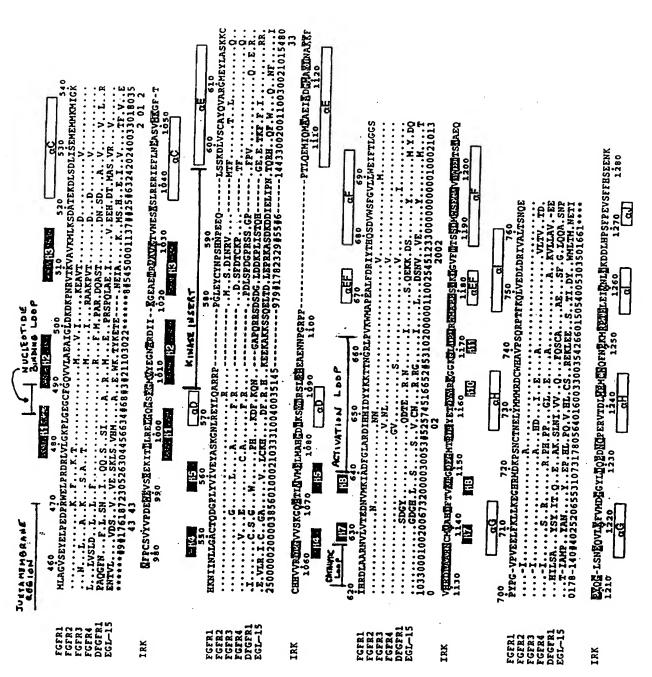
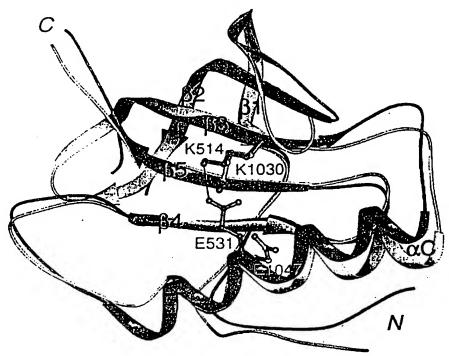


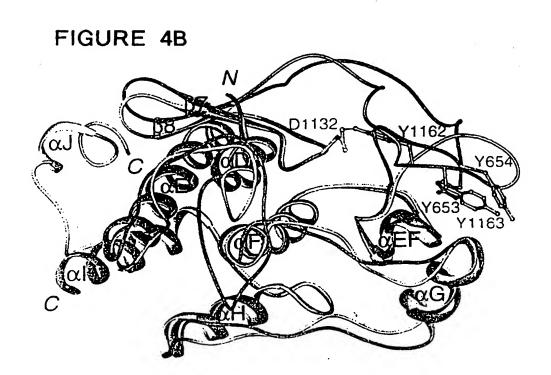
FIGURE 2











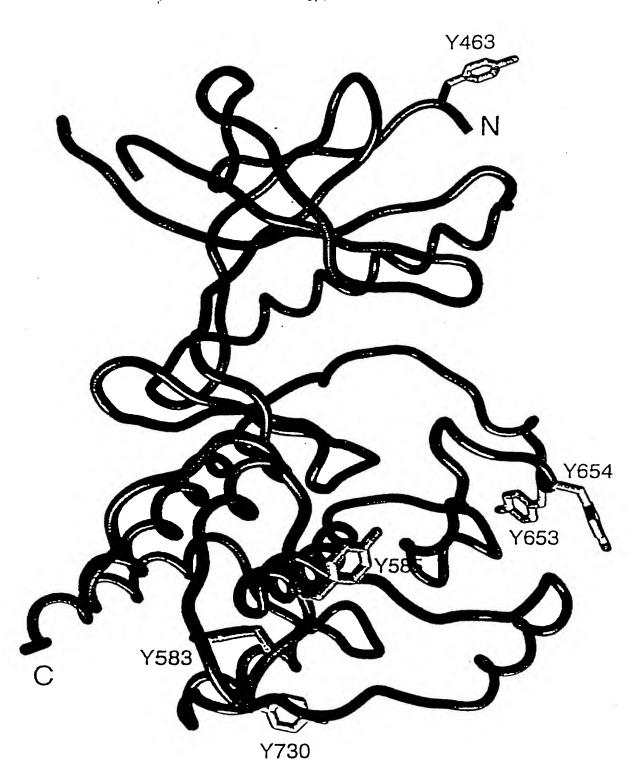


FIGURE 5

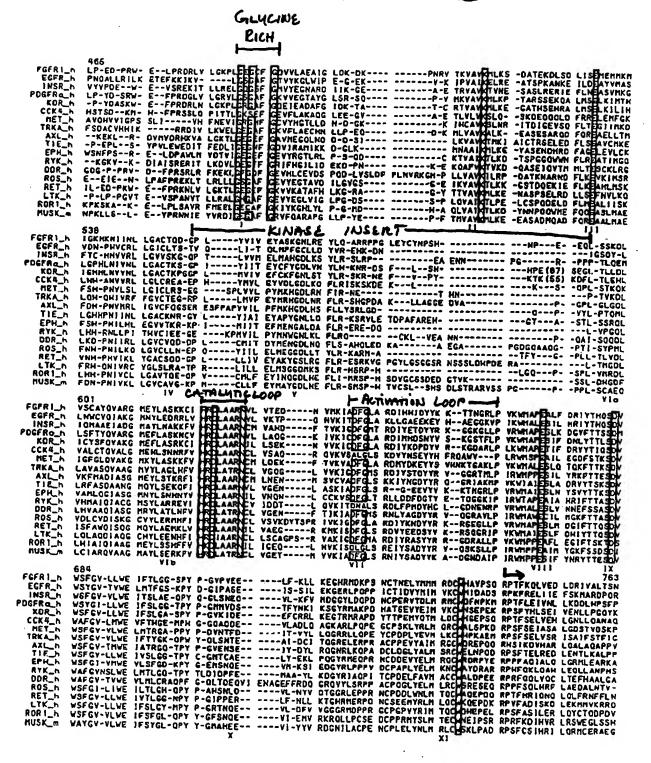


FIGURE 6A

FGFR1_h	105 10FOPRUFIP	RORI VI CX-P	BEREBOYV	LAEAIGLDKD	KPNRVTKVAV	KHLKSDATEK	DLSDLISEME   -EAFLQ-E -QQMLQSE -DEFIE-E -QAFL-AE -EEFLK-E KADTEEMHRE LKAK-FLQ-E GNH1AOLKKE PFAMOOFIRE	MMKHI-GKHK
SRC_h	GLAKDAWEIP	RESLRLEY-K	THE FEVY	MGTW	NGT TRVAT	KILKPGTHSP	-CAFLQ-E	AGAWKKTKHE
BRK_h	LPHYDDWERP	REEFTLCR-K	THE FEET OF	ECLW	PCOYDVAI	KHIKEGSHSE	-DEFIE-E	AKVMMNLSHE
BTK_h	GLGYGSWEID	PKOLTFLK-E	THE PLANT	I CDY	RGNKVAV	KEIKNDA-TA	-QAFL-AE	ASVMTQLRHS .
CSK_h ABL_h	SPNYOKWEME	RTOITHKH-K	LEGETY	EGYW	K-KYSLTVAV	KILKEDTHEY	-EEFLK-E	AAVHKEIKHP
ZAP70_h	LKOKKLF-LK	RONLLIADIE	L PENF SYR	QGYYRM	RKKQ-IDVAL	KALKOG1E	KADTEENRE	MUTUHULUNP
· FES_h	AVPKOKWYLN	HEDLYLCE-0	PREFERENCE	SGR	CKAUNILVAA	KICKNCTS	DSVREKFLOE	ALTHROFOHP
FAK_h JAK1_h	MPSIRDYEIG	RERIELGRC-	I ELLEVE	LCRYDP	EDNTGEOVAV	KELKPE SG	DSVREKFLOE A	TEILANLYHE
ACK_h	PLOSLTCLIG	EKDLRLLE-K	LEDEFEVER	RGEVDA	COUNTRY	KELKPOVESO	PEAMODFIRE	VNAMHSLDHR
	, 1001		1		11		111	
	543							
FGFR1_h	T	-ODEP-LYVI	VEYASKONLR	EYLOARRPPG	LEYCYNPSHN	PEEOLSSKOL	VSCAYQVARG N	MEYLASKKCI
SRC_h	KLYQLYAVVS	-E-EB-141A	TEYHSKGSLL	DELKGET		-CKILKLPUL	1 DIAVOVAEC I	ACAI COUNAI
BRK_h	HILALYAVVS	VG-DP-VYII	TELMAKGSLL	ELLRDSD		-RHRFOTOOL	LEHCKOVCEA !	MEYLESKOFL
BTK_h CSK_h	KEAGEAGACL	KOK-b-ftll	TEYMAKGSLV	DYLRSRG		-RSYLGGDCL	LKFSLDYCEA !	MEYLEGNNFY
ABL_h	NLVQLLGVCT	REP-P-FYII	TEFHTYGNLL	DYLRECH		-ROEVNAVYL	LEHCKOVCEA ! LKFSLOVCEA ! LYNATQISSA !	MEYLEKKNFI
ZAP7O_h	YIVRLIGYCO	AEALMLY	HENACGGPLH	KFLVGK		-REELPVSNV	ILYAYOLSTA E LOMYGDAAAG E LECHOYSHG E	MEYLESKOCI
FES_h	NIVRLIGVCT	-QKQP-IYIV	MELYOGGUPL	SELOVR		-KYSLOLASL	ILYAYOLSTA (	LAYLESKREV
FAK_h JAK 1_h	HIVKLIGVII	EUGGNGIK! [	MEFLPSGSLK	EYLPKN		-KNKINLKQQ	LKYAVOICKG	HDYLGSROYY
ACK_h	NLIRLYGYYL	TPPMKMV	TELAPLGSLL	DRLRKH	• • • • • • • • • • • • • • • • • • • •	GOIN PROIL	SRYAVQVAEG I	
	IV		V			. Via		VIb
			•					
	621		AS L					
FGFR1 h	621 HRDLAARSVL	VTEONVMKIA	AS L	HIDYYKKTTN	GRLPVKWHAP	EAL-FORIYT	HOSDIVWSFGV L	LLWEIFTLGG
FGFR1_h SRC_h	HROLRAADL	VTEDNVMK I A VGENLVCKVA	AS L	HIDYYKKTTN DNEYTARQGA	GRLPYKWHAP -KFPIKWTAP	EAL-FORIYT EAALYGR-FT	HOSDVWSFGV LIKSDVWSFG! L	LLWEIFTLGG LLTELTTKGR
SRC_h BRK_h	HROLRAAR HEL	VTEDNYMK I A VGENLVCKYA VGENTLCKYA	DFG AROIH- DFG ARLIE-	HIDYYKKITN ONEYTARQGA EDYYLSHD-H			HOSDVWSFGV L IKSDVWSFGI L TKSDVWSFGI L SKSDIWAFGV L	LLWEIFTLGG LLTELTTKGR LLHENFSRGO LNWEIYSLGK
SRC_h BRK_h BTK_h	HROLAAR OL HROLAAR OL HROLAAR OL	VNDQCVVKVS	DFG_ARDIH- DFG_ARLIE- DFG_ARLIK- DFG_SRYVL-	-FASSTODTG		ENLITSK-FS	TKSDVVSFGI	LWEIYSFGR
SRC_h BRK_h BTK_h CSK_h	HROLRAARIL HROLAARICL HROLAARICL HROLAARICL HROLAARICL	VNDQCVVKVS VGENHLVKVA	DFG_ARDIH- DFG_ARLIE- DFG_SRYVL- DFG_SRYVL- DFG_SRIMI-	-EASSTODTG GOTYTAHAGA		ENLITSK-FS	TKSDVVSFGI	LWEIYSFGR
SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h	HROLRAARIEL HROLAARIEL HROLAARIEL HROLAARIEL HROLAARIEL HROLAARIEL	VNDQCVVKVS VSEDNVAKVS VGENHLVKVA LVNRHYAKIS	DFG_AROIH- DFG_ARLIE- DFG_ARLIK- DFG_SRYVL- DFG_SKAUGA DFG_SKAUGA	DDEYTSSVGS -EASSTODTG GOTYTAHAGA DDSYYTARSA	-KEPVRWSPP -KLPYKWTAP -KEPIKWTAP GKWPLKWYAP	EALREKK-FS ESLAYNK-FS ECINFRK-FS EN NYCR-YS	TKSDVVSFGI	LWEIYSFGR
SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h	HROLRAARUL HROLAARUL HROLAARUL HROLAARUL HROLAARUL HROLAARUL	VNDQCVVKVS VSEDNVAKVS VGENHLVKVA LVNRHYAK1S VTEKNVLK1S	DFG_ARDIH- DFG_ARLIE- DFG_ARLIK- DFG_SRYVL- DFG_SKALGA DFG_SKALGA DFG_SREEA-	DDEYTSSVGS -EASSTODTG GOTYTAHAGA DDSYYTARSA DGYYAASGGS	-KEPVRWSPP -KLPYKWTAP -KEPIKWTAP GKWPLKWYAP RQYPYKWTAP	EALREKK-FS ESLAYNK-FS ECINFRK-FS EALNYGR-YS	TKSDWAFGI L IKSDWAFGI L SKSDWAFGI L SESDWAFGI L	LWEIYSFGR LWEIATYGH FHWEALSYGO FHWEITSLGA
SRC_h BRK_h BTK_h CSK_h ABL_h ZAP7O_h FES_h FAK_h	HROLRAAMIL HROLAARVIL HROLAARVIL HROLAARVIL HROLAARVIL HROLAARVIL HROLAARVIL HROLAARVIL	VNDQCVVKVS VSEDNVAKVS VGENHLVKVA LVNRHYAK1S VTEKNVLK1S	DFG_ARDIH- DFG_ARLIE- DFG_ARLIK- DFG_SRYVL- DFG_SKALGA DFG_SKALGA DFG_SREEA-	DDEYTSSVGS -EASSTODTG GOTYTAHAGA DDSYYTARSA DGYYAASGGS	-KEPVRWSPP -KLPYKWTAP -KEPIKWTAP GKWPLKWYAP RQYPYKWTAP	EALREKK-FS ESLAYNK-FS ECINFRK-FS EALNYGR-YS	TKSDWAFGI L IKSDWAFGI L SKSDWAFGI L SESDWAFGI L	LWEIYSFGR LWEIATYGH FHWEALSYGO FHWEITSLGA
SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h	HROLRAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROV HROLAAROV HROLAAROV	VNDQCVVKVS VSEDNVAKVS VGENHLVKVA LVNRHYAK1S VTEKNVLK1S	DFG_AROIH- DFG_ARLIE- DFG_ARLIE- DFG_SRYVL- DFG_SKAUT- DFG_SKAUGA DFG_SKAUGA DFG_SKYME- DFG_TKAIET DFG_MRALPO	DDEYTSSVGS -EASSTODTG GOTYTAHAGA DDSYYTARSA DGYYAASGGS	-KFPVRWSPP -KLPVKWTAP -KFPIKWTAP CKWPLKWYAP RQYPVKWTAP GKLPIKWMAP RDSPVFWYAP RKVPFAWCAP	EALHTSK-FS EALHEKK-FS ESLAYNK-FS ESLNYGR-YS EALNYGR-FT ESLHOSK-FY ESLKTRT-FS	TKSDVVSFGI L IKSDVVSFGI L SRSDVVSFGI L SESDVVSFGI L SASDVVMFGV I HASDIVMFGV I	LWEIYSFGR LWEIATYGH FHWEALSYGO FHWEITSLGA
SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h FAX_h JAK1_h	HROLRAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROL HROLAAROV HROLAAROV HROLAAROV	VNDQCVVKVS VSEDNVAKVS VGENHLVKVA LVNRHVAKIS VIEKNVLKIS VSSNDCVKLG VESEHQVKIG	DFG_ARDIH- DFG_ARLIE- DFG_ARLIK- DFG_SRYVL- DFG_SKALGA DFG_SKALGA DFG_SREEA-	DDEYTSSVGS -EASSTODTG GOTYTAHAGA DDSYYTARSA DGYYAASGGS	-KFPVRWSPP -KLPVKWTAP -KFPIKWTAP CKWPLKWYAP RQYPVKWTAP GKLPIKWMAP RDSPVFWYAP RKVPFAWCAP	EALREKK-FS ESLAYNK-FS ECINFRK-FS EALNYGR-YS	TKSDWAFGI L IKSDWAFGI L SKSDWAFGI L SESDWAFGI L	LLWEITSFGR LLWEITSFGR INWEALSTGO LLWETFSLGA CHWEILMHGV ILHELLTYCD ILWEHFTYGO
SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h FAX_h JAK1_h	HROLAAR VIL HROLAAR VIL HROLAAR VIL HROLAAR VIL HROLAAR VIL HROLAAR VIL HROLAAR VIL HROLAAR VIL HROLAAR VIL HROLAAR VIL	VNDQGVVKVS VSEDNVAKVS VGENHLVKVA LVNRHYAKIS VIEKNVLKIS VESEHQVKIG LATROLVKIG LATROLVKIG	DFG_ARDIH- DFG_ARLIE- DFG_ARLIK- DFG_SRYVL- DFG_SKALGA DFG_SKALGA DFG_SKALGA DFG_SKALGA DFG_SKYME- DFG_TKAIET DFG_MRALPO VII	DDEYTSSVGS -EASSTODGA GDTYTAHAGA DDSYYTARSA DGVYAASGGS DSTYYKA-SK OKEYYTVKDD NODHYVHOEH	-KFPVRWSPP -KLPVKWTAP -KFPIKWTAP CKWPLKWYAP RQVPVKWTAP GKLPIKWTAP ROSPVFWYAP RKVPFAWCAP	ENLITSK-FS EALREKK-FS EELAYNK-FS EELINFRK-FS EALNYGR-YS ESINFRR-FT EELHOSK-FY EELKTRT-FS VIII	TKSDVWSFGI I IKSDVWSFGV I SRSDVWSYGC I SESDVWSFGI I SASDVWHFGV I IASDVWSFGV I HASDIVMFGV I	LIVETYSFGR LLVETATYGM FNVEALSYGO LLVETFSLGA CHVETFHGV FLHELLTYCD FLWENFTYGO
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FIGURE 6B

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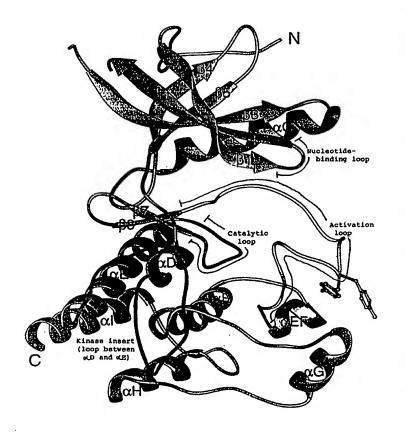
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#### (57) Abstract

The present invention relates to the three-dimensional structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates that define the structures of the protein tyrosine kinase and any of the compounds bound to it are pertinent to methods for determining the three-dimensional structures of protein tyrosine kinases with unknown structure and to methods that identify modulators of protein tyrosine kinase functions.



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### DESCRIPTION

#### CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

5 <u>RELATED APPLICATIONS</u>

This application is related to U.S. Application Serial No. 08/701,191, by Mohammadi, et al., entitled "Crystals of the Tyrosine Kinase Domain of Non-Insulin Receptor Tyrosine Kinases," filed August 21, 1996 (Lyon & Lyon Docket No. 227/088) and U.S. Application Serial No. 60/034,168, by McMahon, et al., entitled "Crystal Structures of a Protein Tyrosine Kinase Complexed with Compounds of the Oxindolinone/Thiolindolinone Family," filed December 19, 1996 (Lyon & Lyon Docket No. 221/282), which are hereby incorporated herein by reference in their entirety including any drawings, tables, and figures.

### INTRODUCTION

The present invention relates to the three dimensional structures of protein kinases.

# BACKGROUND OF THE INVENTION

The following description of the background of the invention is provided simply as an aid in understanding the invention and is not admitted to describe or constitute prior art to the invention.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes (for a review, see Schlessinger and Ullrich, 1992, Neuron 9: 383-391). The PTK family contains multiple subfamilies, one of which

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is the fibroblast growth factor receptor (FGF-R) subfamily (for a review, see Givol and Yayon, 1992, FASEB J. 6 (15): 3362-3369).

All PTKs enzymatically transfer a high energy phosphate from adenosine triphosphate to a tyrosine residue in a target protein. These phosphorylation events regulate cellular phenomena in signal transduction processes. Cellular signal transduction processes contain multiple steps that convert an extracellular signal into an intracellular signal. intracellular signal is then converted into a cellular response. PTKs are components in many signal transduction processes. A PTK regulates the flow of a signal in a particular step in the process by phosphorylating a downstream molecule. The addition of a phosphate can either modulate the activity of the downstream molecule by turning it "on" or "off". Thus, aberrations in a particular PTK's activity can either cause overflow or underflow of the signal. Overflow of a signal can lead to such abnormalities as uncontrolled cell proliferation, which is representative of such disorders as cancer and angiogenesis.

Scientists in the biomedical community are searching for PTK inhibitors that down-regulate overflow signal transduction pathways. In particular, small molecule PTK inhibitors are sought that can traverse the cell membrane and not become hydrolyzed in acidic environments. These small molecule PTK inhibitors can be highly bioavailable and can be administered orally to patients.

Some small molecule PTK inhibitors have already

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been discovered. For example, bis(monocyclic), bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808), 1-cyclopropyl-4-pyridyl-quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 A1), seleoindoles and selenides (PCT WO 94/03427), tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although many PTK inhibitors are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the indolinone family, however, are specific for the FGFR subfamily and are non-hydrolyzable. WO 96/40116, "Indolinone Compounds for the Treatment of Disease," published December 19, 1996, inventors Tang et al. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, they are not complexed with PTK subfamily specific, hydrolysis resistant, small molecules.

Despite recent advances, the need remains in the art for crystallographic analysis of protein kinases, so that improved therapeutic molecules can be designed and synthesized.

## SUMMARY OF THE INVENTION

The present invention relates to the three

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dimensional structures of protein tyrosine kinases. The use of X-ray crystallography can define the three dimensional structure of protein tyrosine kinase at atomic resolution.

The three dimensional structures described herein elucidate specific interactions between protein tyrosine kinases and compounds bound to them. The coordinates that define the three dimensional structures of protein tyrosine kinases are useful for determining three dimensional structures of PTKs with unknown structure. In addition, the coordinates are also useful for designing and identifying modulators of protein tyrosine kinase function. These modulators are potentially useful as therapeutics for diseases, including (but limited to) cell proliferative diseases, such as cancer, angiogenesis, atherosclerosis, and arthritis.

Thus in a first aspect, the invention features a crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

The term "crystalline form," in the context of the invention, is a crystal formed from an aqueous solution comprising a purified polypeptide corresponding to the catalytic domain of a PTK. A crystalline form of a protein tyrosine kinase is characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al., 1976, Protein Crystallography, Academic Press. A crystalline form of a protein kinase is not characterized as being capable of diffracting x-rays in a pattern analogous to a crystalline form consisting of primarily salt or primarily a compound, for example.